Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 11:57 pm GMT

PDB ID	:	5FQ6
Title	:	Crystal structure of the SusCD complex BT2261-2264 from Bacteroides thetaiotaomicron
Authors	:	Glenwright, A.J.; Pothula, K.R.; Chorev, D.S.; Basle, A.; Robinson, C.V.; Kleinekathoefer, U.; Bolam, D.N.; van den Berg, B.
Deposited on	:	2015-12-07
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

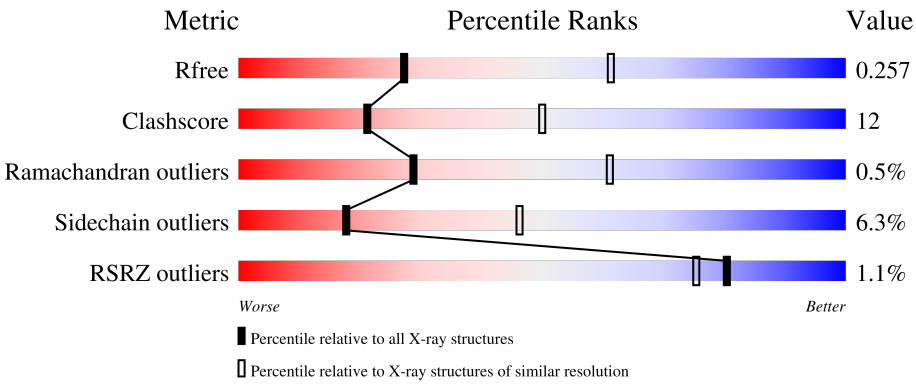
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	72% 26% •
1	C	480	77% 22% •
1	H	480	% 70% 26% •
1	L	480	% 61% 35% •

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Mol	Chain	Length	Quality of chain
2	B	984	% 66% 27%
2	D	984	% 72% 21%
2	I	984	% 71% 23%
2	M	984	% 71% 23%
3	E	148	% 80% 17%
3	F	148	5% 70% 28%
3	J	148	2% 70% 26%
3	N	148	6% 62% 34%
4	G	10	10% 80% 20%
4	K	10	80% 20%
4	O	10	10% 60% 40%
4	P	10	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 49282 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PUTATIVE LIPOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	3749	2373	616	743	17	0	1	0
1	C	480	3749	2373	616	743	17	0	1	0
1	H	480	3749	2373	616	743	17	0	1	0
1	L	480	3749	2373	616	743	17	0	1	0

- Molecule 2 is a protein called SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	941	7326	4635	1222	1439	30	0	0	0
2	D	945	7359	4658	1226	1445	30	0	0	0
2	I	947	7374	4665	1230	1449	30	0	0	0
2	M	948	7383	4670	1231	1452	30	0	0	0

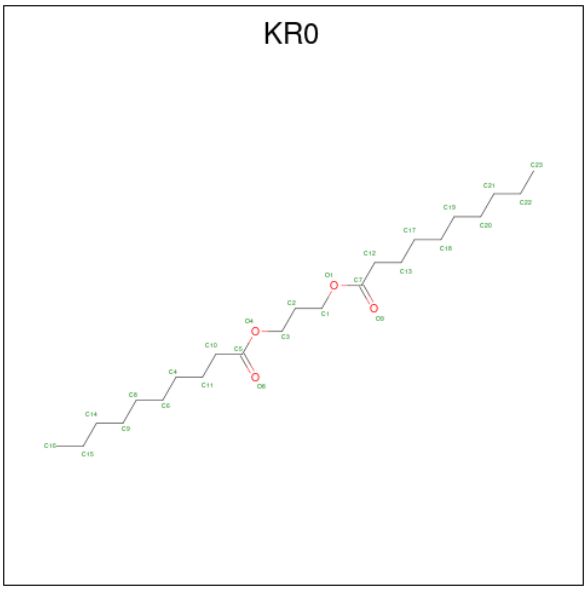
- Molecule 3 is a protein called UNCHARACTERIZED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	146	1142	721	180	236	5	0	0	0
3	F	146	1142	721	180	236	5	0	0	0
3	J	146	1142	721	180	236	5	0	0	0
3	N	146	1142	721	180	236	5	0	0	0

- Molecule 4 is a protein called BT_2261.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	10	40	20	10	10	0	0	0
4	K	10	40	20	10	10	0	0	0
4	O	10	40	20	10	10	0	0	0
4	P	10	40	20	10	10	0	0	0

- Molecule 5 is 3-decanoyloxypropyl decanoate (three-letter code: KR0) (formula: $C_{23}H_{44}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	27	23	4	0	0
5	D	1	27	23	4	0	0
5	I	1	27	23	4	0	0
5	M	1	27	23	4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	B	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	D	1	1	1	0	0
			Total	Na		
6	I	1	1	1	0	0
			Total	Na		
6	M	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

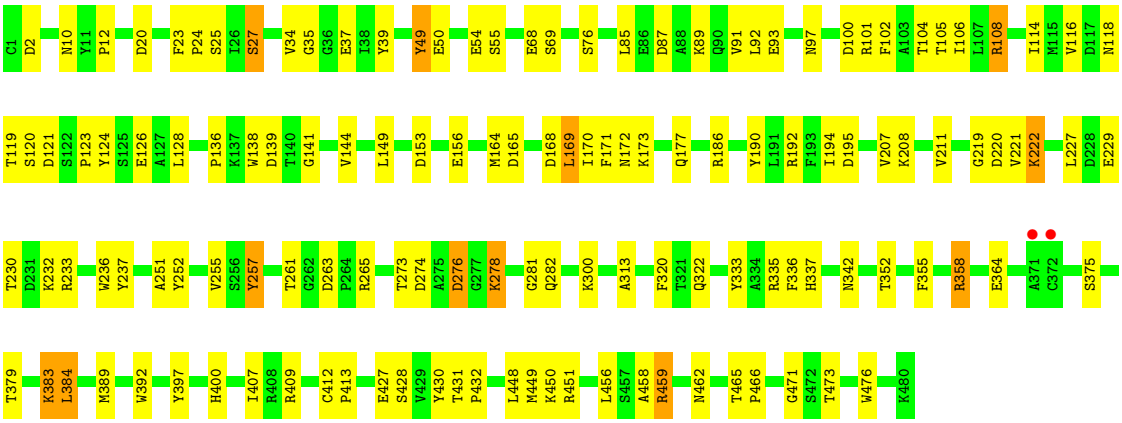
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	B	1	1	1	0	0
			Total	Ca		
7	D	1	1	1	0	0
			Total	Ca		
7	I	1	1	1	0	0
			Total	Ca		
7	M	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

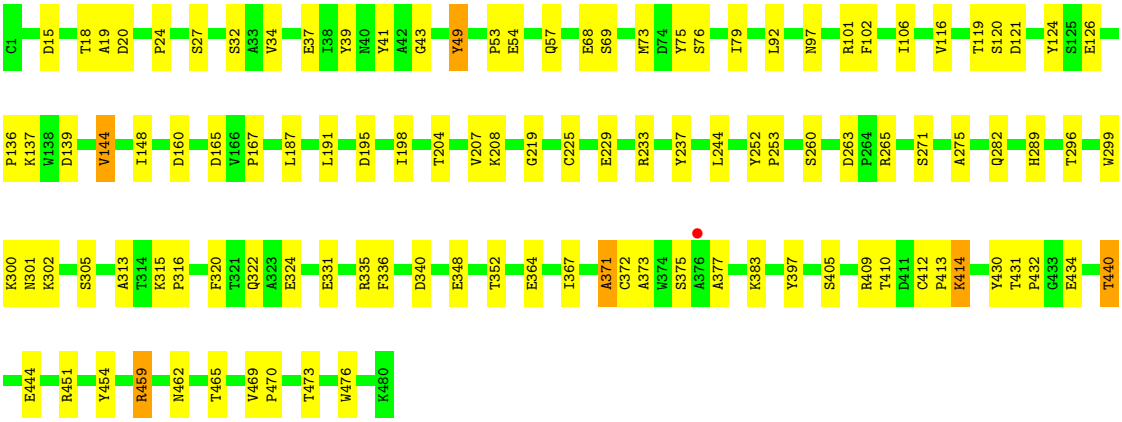
• Molecule 1: PUTATIVE LIPOPROTEIN

Chain A: 72% 26%



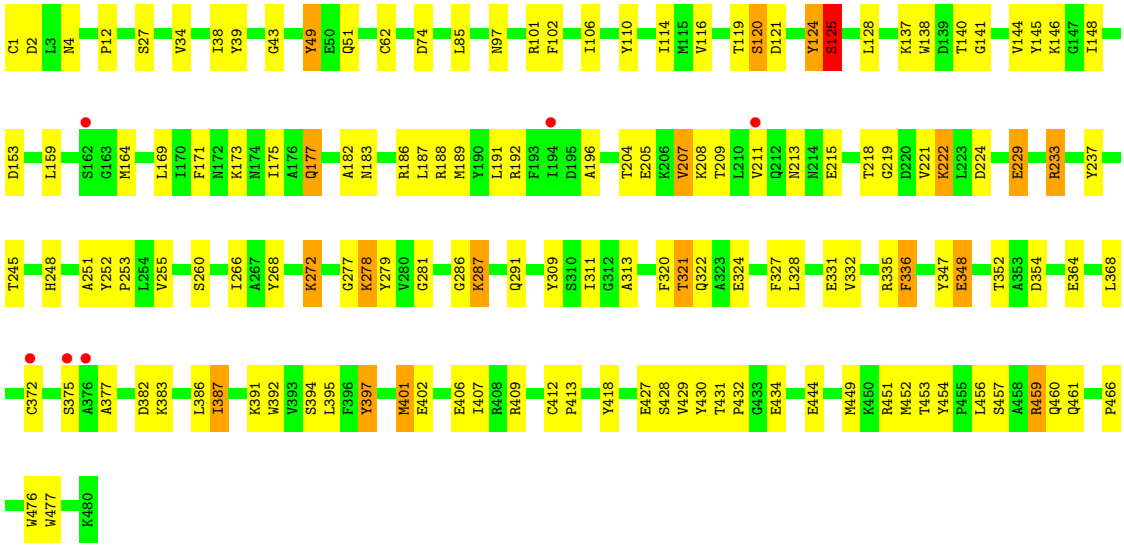
• Molecule 1: PUTATIVE LIPOPROTEIN

Chain C: 77% 22%



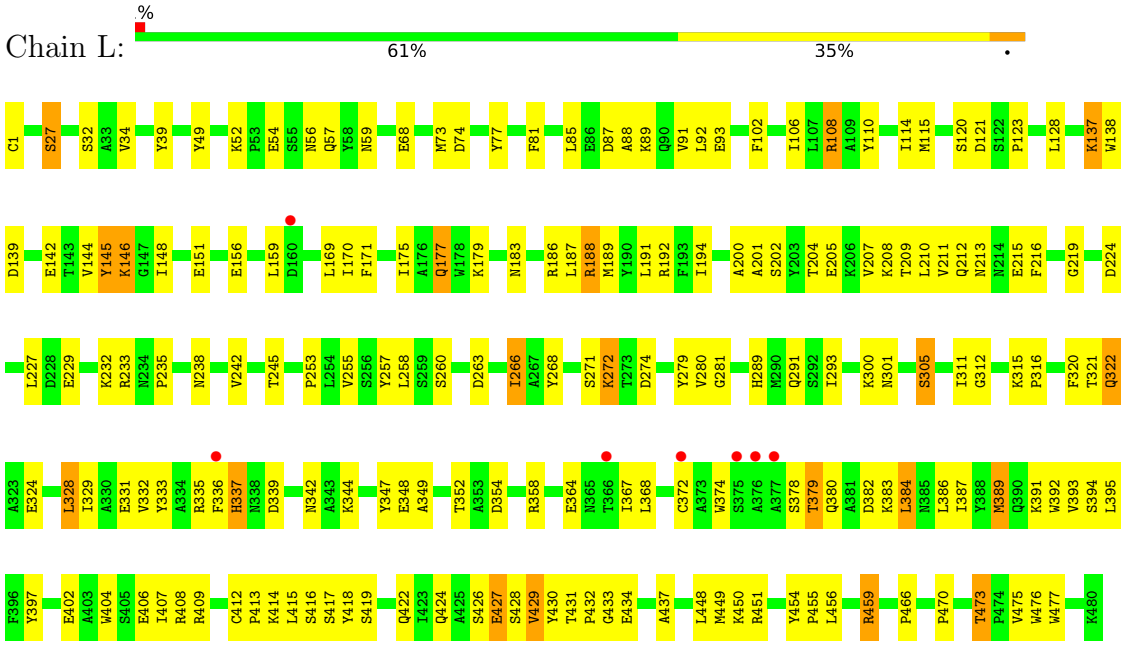
• Molecule 1: PUTATIVE LIPOPROTEIN

Chain H: % 70% 26%



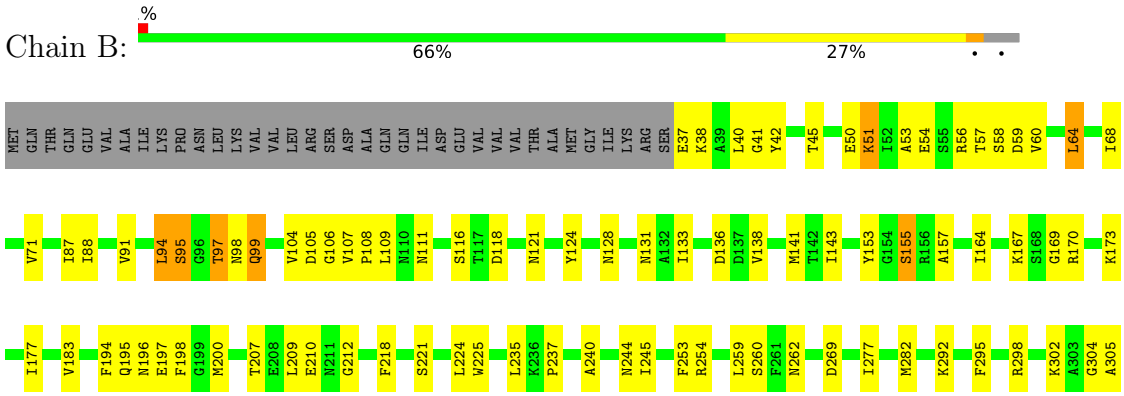
- Molecule 1: PUTATIVE LIPOPROTEIN

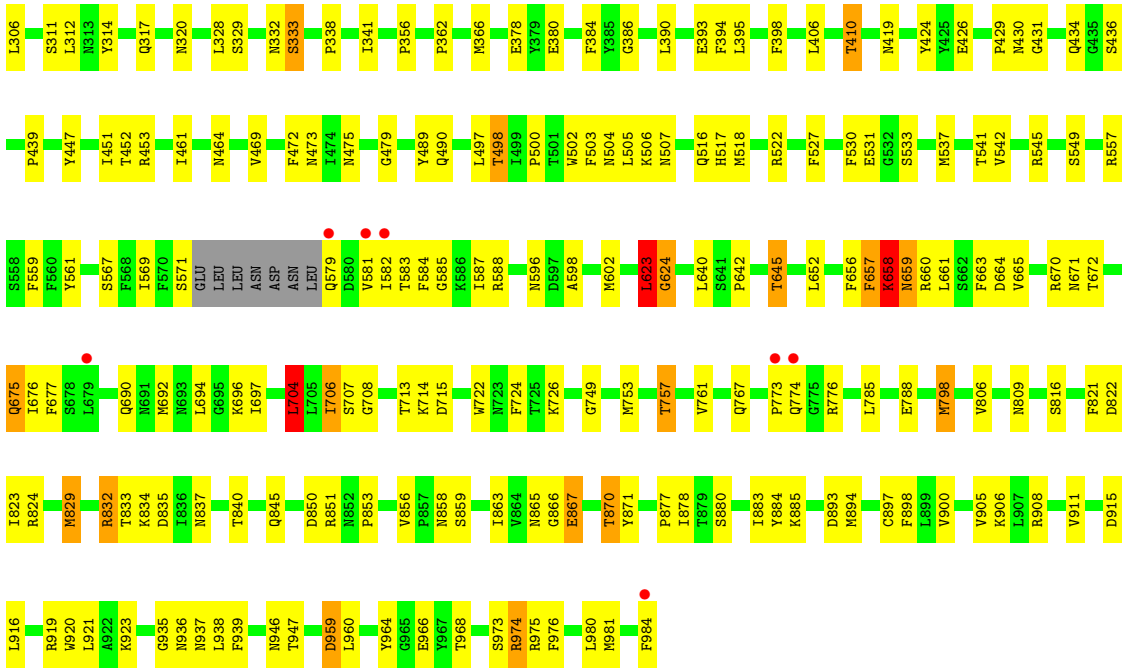
Chain L:



- Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

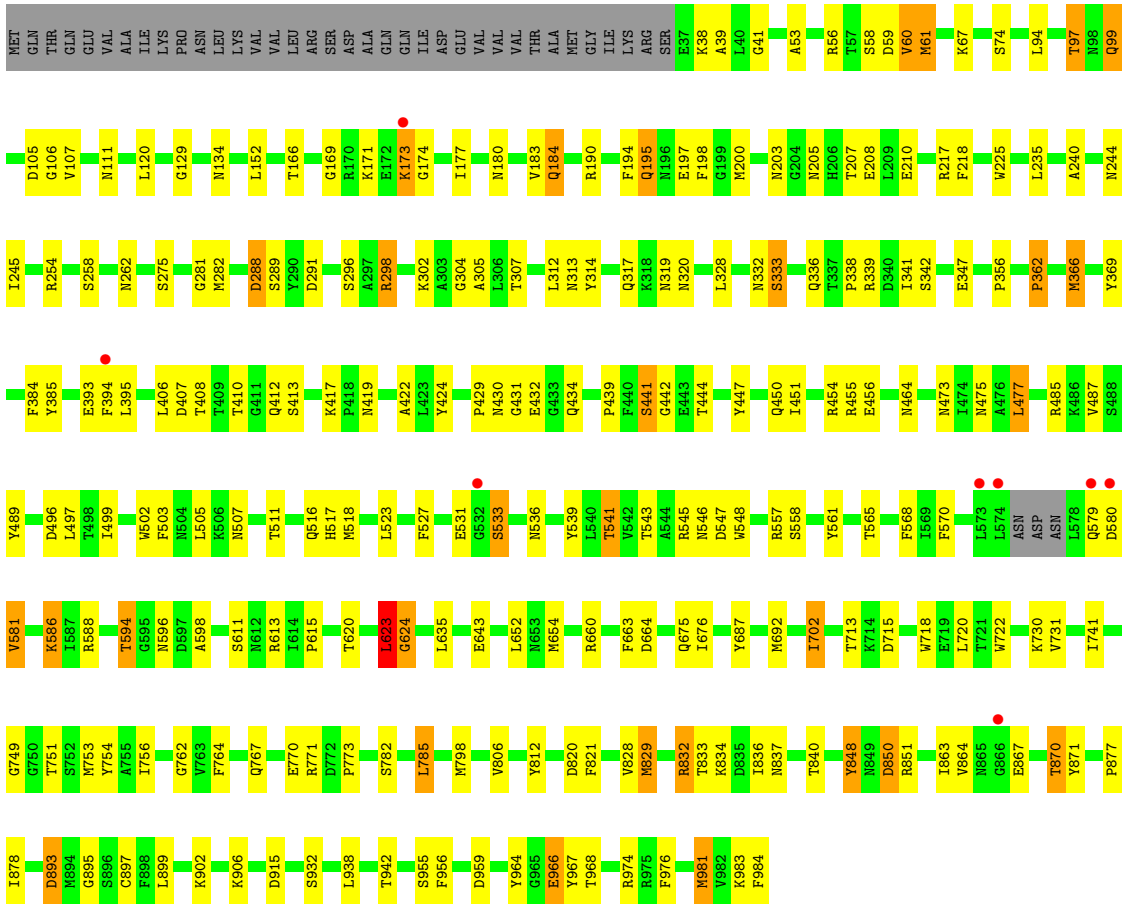
Chain B:





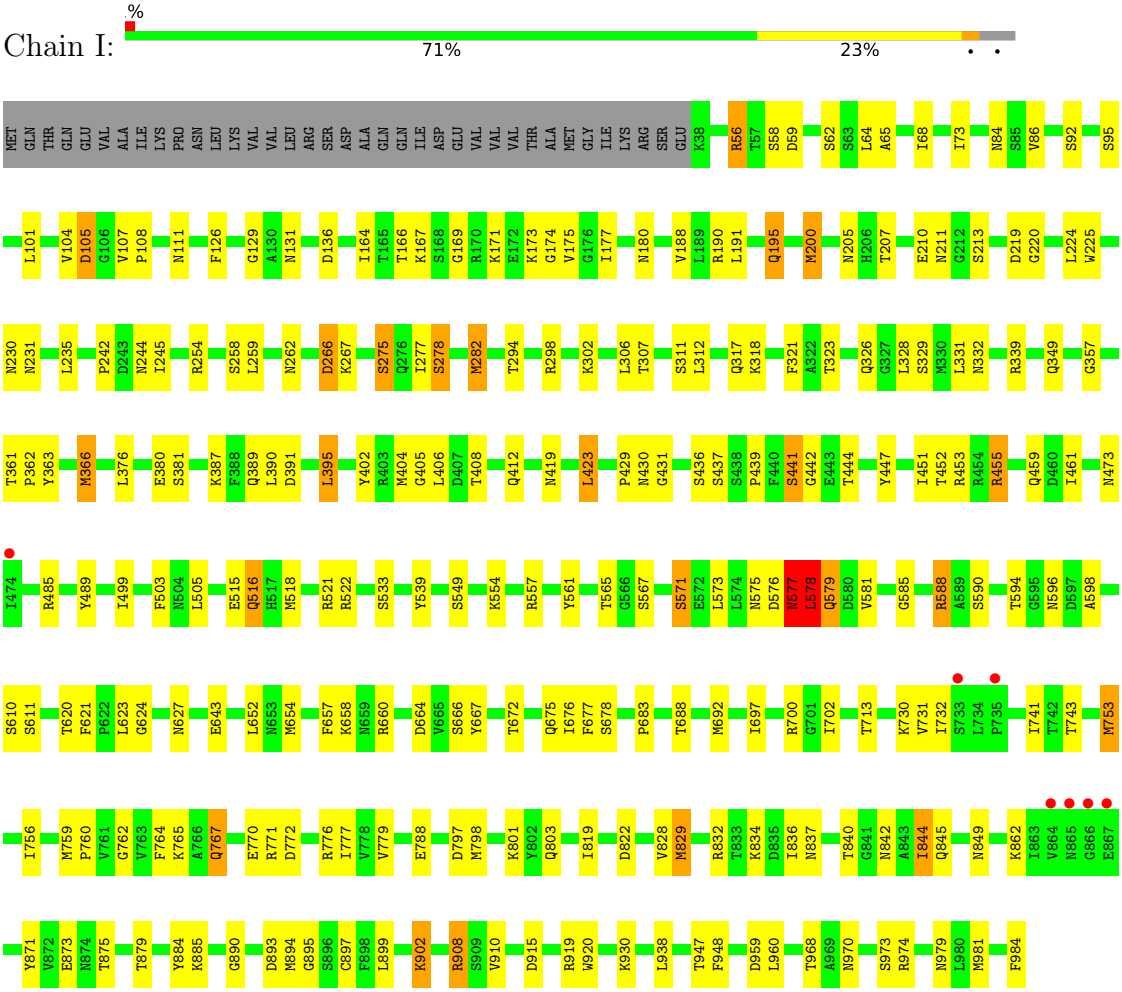
• Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

Chain D:



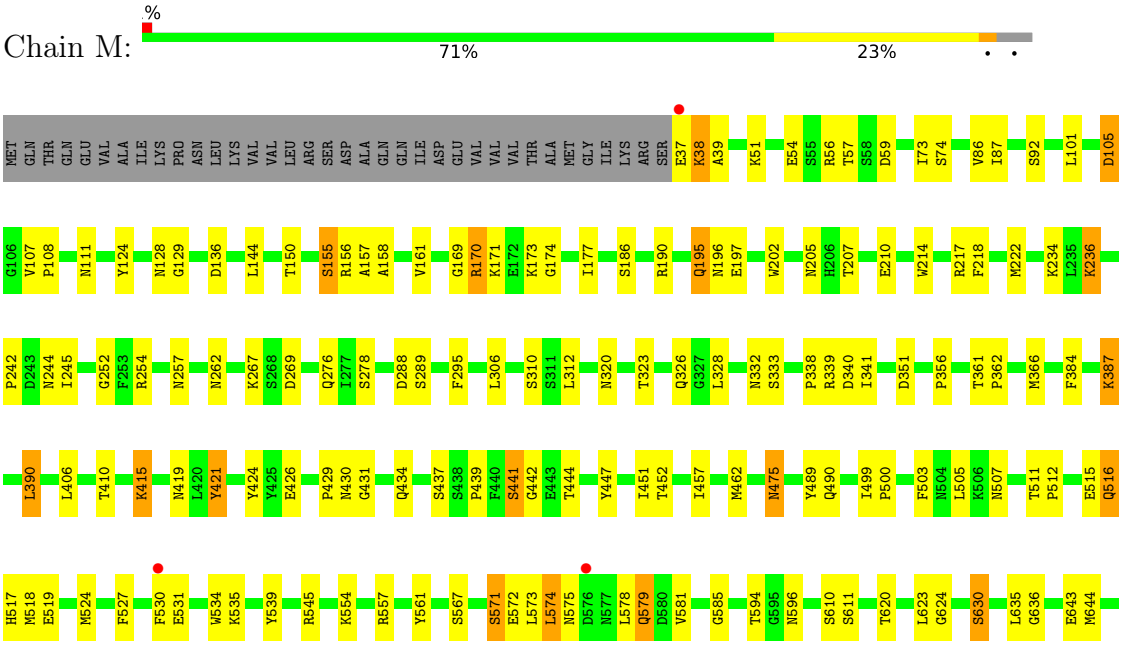
• Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

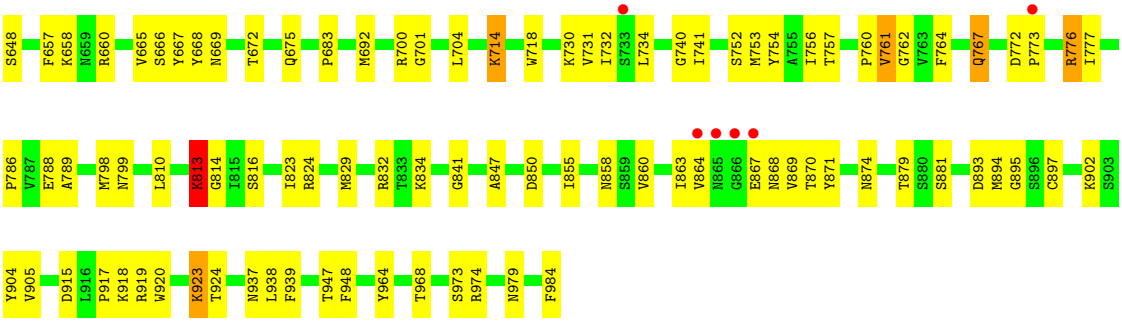
Chain I:



• Molecule 2: SUSC/RAGA FAMILY TONB-LINKED OUTER MEMBRANE PROTEIN

Chain M:



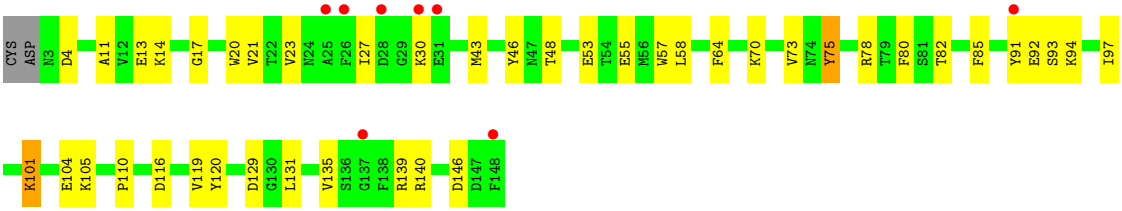


- Molecule 3: UNCHARACTERIZED PROTEIN

Chain E:

- Molecule 3: UNCHARACTERIZED PROTEIN

Chain F:

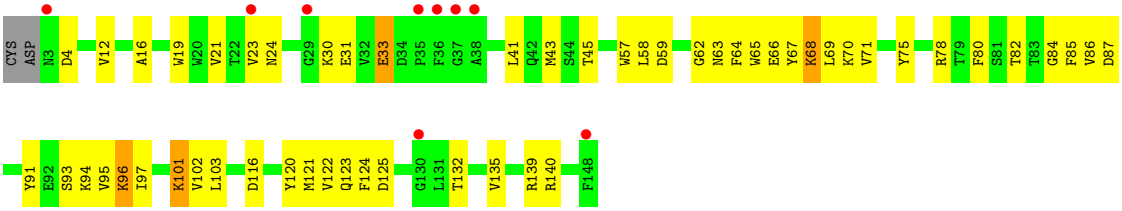


- Molecule 3: UNCHARACTERIZED PROTEIN

Chain J:

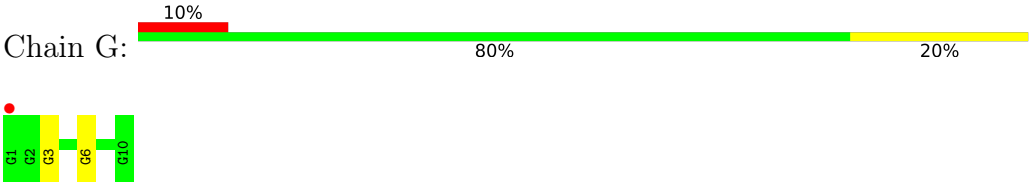
- Molecule 3: UNCHARACTERIZED PROTEIN

Chain N:



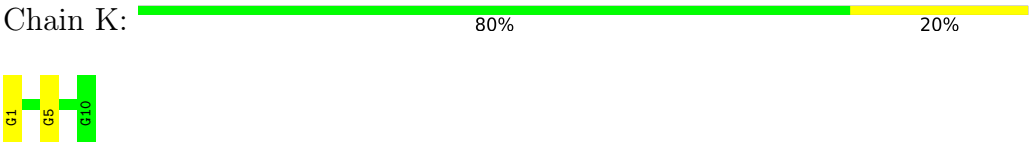
• Molecule 4: BT_2261

Chain G:



• Molecule 4: BT_2261

Chain K:



• Molecule 4: BT_2261

Chain O:

• Molecule 4: BT_2261

Chain P:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	222.03Å 91.94Å 261.22Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	48.80 – 2.80 48.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.80-2.80) 91.5 (48.80-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.255 0.200 , 0.257	Depositor DCC
R_{free} test set	10274 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	1.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49282	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8863e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NA, KR0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.42	0/3843	0.56	0/5231
1	C	0.41	0/3843	0.59	0/5231
1	H	0.42	0/3843	0.59	0/5231
1	L	0.43	0/3843	0.59	0/5231
2	B	0.44	0/7503	0.65	6/10176 (0.1%)
2	D	0.45	1/7536 (0.0%)	0.68	3/10221 (0.0%)
2	I	0.45	0/7552	0.68	4/10245 (0.0%)
2	M	0.46	0/7561	0.67	4/10257 (0.0%)
3	E	0.42	0/1170	0.62	0/1589
3	F	0.40	0/1170	0.59	0/1589
3	J	0.38	0/1170	0.60	0/1589
3	N	0.39	0/1170	0.60	0/1589
4	G	0.55	0/39	1.23	0/47
4	K	0.53	0/39	0.77	0/47
4	O	0.52	0/39	0.86	0/47
4	P	0.57	0/39	0.70	0/47
All	All	0.44	1/50360 (0.0%)	0.64	17/68367 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	H	0	1
1	L	0	2
2	B	0	2
2	D	0	1
2	I	0	2
2	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	850	ASP	CB-CG	5.11	1.62	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	624	GLY	N-CA-C	-8.59	91.64	113.10
2	I	624	GLY	N-CA-C	-7.58	94.16	113.10
2	D	850	ASP	CB-CG-OD1	7.13	124.72	118.30
2	I	578	LEU	CA-CB-CG	7.11	131.66	115.30
2	B	64	LEU	CB-CG-CD1	-6.70	99.61	111.00
2	D	624	GLY	N-CA-C	-6.63	96.53	113.10
2	B	704	LEU	CA-CB-CG	6.54	130.35	115.30
2	B	757	THR	C-N-CA	-6.47	108.72	122.30
2	D	623	LEU	CA-CB-CG	5.99	129.09	115.30
2	B	624	GLY	N-CA-C	-5.95	98.22	113.10
2	B	623	LEU	CA-CB-CG	5.85	128.75	115.30
2	M	573	LEU	CA-CB-CG	5.67	128.35	115.30
2	M	850	ASP	CB-CG-OD1	5.59	123.33	118.30
2	I	577	ASN	N-CA-C	5.27	125.23	111.00
2	B	850	ASP	CB-CG-OD1	5.14	122.93	118.30
2	I	395	LEU	CA-CB-CG	5.14	127.12	115.30
2	M	105	ASP	N-CA-C	5.12	124.81	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	37	GLU	Peptide
2	B	623	LEU	Peptide
1	C	336	PHE	Peptide
2	D	623	LEU	Peptide
1	H	336	PHE	Peptide
2	I	266	ASP	Peptide
2	I	623	LEU	Peptide
1	L	336	PHE	Peptide
1	L	337	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	M	38	LYS	Peptide
2	M	623	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3749	0	3566	90	0
1	C	3749	0	3566	72	0
1	H	3749	0	3566	106	0
1	L	3749	0	3566	146	0
2	B	7326	0	6994	196	0
2	D	7359	0	7033	151	0
2	I	7374	0	7044	160	0
2	M	7383	0	7050	160	0
3	E	1142	0	1056	17	0
3	F	1142	0	1056	27	0
3	J	1142	0	1056	25	0
3	N	1142	0	1056	57	0
4	G	40	0	32	1	0
4	K	40	0	32	3	0
4	O	40	0	32	2	0
4	P	40	0	32	0	0
5	B	27	0	0	0	0
5	D	27	0	0	0	0
5	I	27	0	0	0	0
5	M	27	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
7	M	1	0	0	0	0
All	All	49282	0	46737	1162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:VAL:HG21	1:H:332:VAL:HG21	1.51	0.92
3:N:85:PHE:HA	3:N:96:LYS:HE3	1.50	0.92
3:N:68:LYS:NZ	3:N:69:LEU:O	2.03	0.91
2:B:302:LYS:NZ	2:B:304:GLY:O	2.04	0.90
3:N:19:TRP:HE1	3:N:45:THR:HG22	1.35	0.89
2:M:658:LYS:HD2	2:M:660:ARG:HG2	1.55	0.88
1:H:34:VAL:HG11	1:H:114:ILE:HD13	1.55	0.88
1:C:296:THR:HG23	2:D:205:ASN:HD22	1.37	0.87
2:M:328:LEU:HD22	2:M:366:MET:HG3	1.57	0.87
3:N:21:VAL:HG11	3:N:43:MET:HE2	1.57	0.86
2:D:190:ARG:HH12	2:D:942:THR:HG21	1.41	0.86
2:M:864:VAL:HG12	2:M:869:VAL:HA	1.58	0.86
1:L:34:VAL:HG11	1:L:114:ILE:HD13	1.57	0.85
1:C:412:CYS:SG	1:C:414:LYS:NZ	2.50	0.84
2:D:111:ASN:HA	2:D:129:GLY:HA3	1.60	0.84
1:L:192:ARG:HG2	1:L:409:ARG:HD3	1.60	0.84
2:B:207:THR:HG22	2:B:209:LEU:H	1.44	0.83
2:M:920:TRP:O	2:M:923:LYS:NZ	2.10	0.83
1:C:289:HIS:NE2	1:C:440:THR:HG22	1.95	0.82
2:D:833:THR:O	2:D:837:ASN:ND2	2.12	0.82
2:I:361:THR:HG22	2:I:363:TYR:H	1.42	0.81
1:H:245:THR:HG23	2:I:437:SER:HA	1.61	0.81
1:L:451:ARG:NH1	1:L:454:TYR:OH	2.15	0.80
2:M:73:ILE:HG12	2:M:86:VAL:HG22	1.64	0.80
2:B:136:ASP:O	2:B:167:LYS:NZ	2.16	0.78
2:B:195:GLN:NE2	2:B:198:PHE:H	1.82	0.78
2:D:753:MET:HE3	2:D:964:TYR:HA	1.66	0.78
2:D:767:GLN:HG2	2:D:895:GLY:H	1.47	0.78
2:D:837:ASN:HA	2:D:840:THR:HG22	1.66	0.77
2:I:111:ASN:HA	2:I:129:GLY:HA3	1.65	0.77
3:N:84:GLY:O	3:N:96:LYS:HD2	1.84	0.77
2:I:767:GLN:HG2	2:I:895:GLY:H	1.48	0.77
2:I:326:GLN:HE22	4:K:5:GLY:HA2	1.50	0.77
3:F:82:THR:HG22	3:F:97:ILE:H	1.49	0.77
1:L:454:TYR:HE2	1:L:466:PRO:HB2	1.49	0.77
2:D:207:THR:OG1	2:D:210:GLU:HG2	1.84	0.76
2:B:111:ASN:OD1	2:B:128:ASN:ND2	2.19	0.76
2:I:577:ASN:O	2:I:579:GLN:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:16:ALA:HA	3:N:45:THR:HG23	1.69	0.75
2:I:938:LEU:O	2:I:974:ARG:NH1	2.20	0.75
2:M:190:ARG:HH21	2:M:947:THR:HA	1.52	0.75
1:L:137:LYS:NZ	1:L:139:ASP:OD1	2.18	0.75
2:I:205:ASN:OD1	3:J:140:ARG:NH2	2.20	0.74
3:J:48:THR:HG22	3:J:50:SER:H	1.51	0.74
2:I:834:LYS:NZ	2:I:897:CYS:O	2.20	0.74
2:D:60:VAL:HG12	2:D:61:MET:HG2	1.69	0.74
1:H:321:THR:HG22	1:H:324:GLU:HB2	1.66	0.74
2:M:306:LEU:HD11	2:M:390:LEU:HD11	1.70	0.74
1:A:208:LYS:NZ	1:A:336:PHE:O	2.19	0.74
3:F:104:GLU:HG2	3:F:105:LYS:HG2	1.69	0.74
3:F:82:THR:CG2	3:F:97:ILE:H	2.00	0.74
2:I:211:ASN:HB3	2:I:361:THR:HG21	1.70	0.74
2:B:704:LEU:HD12	2:B:724:PHE:HB3	1.70	0.74
2:D:499:ILE:HB	2:D:507:ASN:HD21	1.53	0.73
2:I:56:ARG:HD2	2:I:979:ASN:HD22	1.53	0.73
3:N:57:TRP:HB3	3:N:68:LYS:HE3	1.70	0.73
2:M:879:THR:HG22	2:M:881:SER:H	1.52	0.73
2:B:581:VAL:HG13	2:B:582:ILE:HG12	1.71	0.73
2:M:596:ASN:HB3	2:M:643:GLU:HB3	1.70	0.73
1:H:331:GLU:OE2	1:H:409:ARG:NH2	2.21	0.73
1:H:266:ILE:HG23	1:H:279:TYR:HE2	1.54	0.72
1:L:108:ARG:NH1	1:L:151:GLU:OE1	2.22	0.72
1:H:51:GLN:HB3	1:H:287:LYS:HD2	1.71	0.72
2:B:71:VAL:HG12	2:B:88:ILE:HG12	1.70	0.72
1:L:352:THR:HG22	1:L:364:GLU:HG3	1.69	0.72
2:B:893:ASP:HB2	2:B:897:CYS:HB2	1.71	0.72
1:H:352:THR:HG22	1:H:364:GLU:HG3	1.71	0.72
1:L:207:VAL:HG12	1:L:332:VAL:HG21	1.72	0.72
2:M:571:SER:OG	2:M:585:GLY:N	2.23	0.72
2:B:598:ALA:HB2	2:B:676:ILE:HD12	1.71	0.72
2:D:419:ASN:HD21	2:D:422:ALA:HB3	1.55	0.72
2:I:177:ILE:HB	2:I:984:PHE:HB2	1.72	0.71
2:M:753:MET:HE3	2:M:964:TYR:HA	1.71	0.71
2:M:177:ILE:HB	2:M:984:PHE:HB2	1.72	0.71
2:B:833:THR:O	2:B:837:ASN:ND2	2.23	0.71
2:M:923:LYS:H	2:M:923:LYS:HD3	1.54	0.71
2:D:451:ILE:HG21	2:M:451:ILE:HG21	1.72	0.71
2:B:823:ILE:HG12	2:B:905:VAL:HG22	1.73	0.70
2:I:59:ASP:OD1	2:I:131:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:762:GLY:HA3	2:M:798:MET:HG2	1.73	0.70
1:L:211:VAL:HG21	1:L:332:VAL:HG11	1.74	0.70
1:H:219:GLY:O	1:H:322:GLN:HB2	1.92	0.69
2:B:195:GLN:HE21	2:B:198:PHE:H	1.37	0.69
1:L:213:ASN:HB3	1:L:215:GLU:HG3	1.72	0.69
1:H:4:ASN:OD1	2:I:557:ARG:NH2	2.25	0.69
2:D:579:GLN:HA	2:D:580:ASP:HB3	1.75	0.69
1:L:156:GLU:OE1	1:L:186:ARG:NH2	2.26	0.69
2:B:549:SER:O	2:B:557:ARG:HD3	1.93	0.69
2:I:167:LYS:O	2:I:298:ARG:NH1	2.26	0.69
1:L:110:TYR:CZ	1:L:114:ILE:HD11	2.27	0.69
2:M:205:ASN:OD1	3:N:140:ARG:NH2	2.25	0.69
3:N:85:PHE:HA	3:N:96:LYS:CE	2.22	0.69
1:A:459:ARG:NH2	1:A:466:PRO:O	2.26	0.68
2:D:197:GLU:OE2	2:D:217:ARG:NH1	2.25	0.68
2:B:863:ILE:HB	2:B:870:THR:HG23	1.75	0.68
2:D:430:ASN:O	2:D:439:PRO:HD2	1.93	0.68
2:I:788:GLU:HA	2:I:894:MET:HE1	1.76	0.68
3:J:140:ARG:NH1	3:J:147:ASP:OD1	2.27	0.68
2:B:713:THR:HG22	2:B:715:ASP:H	1.58	0.68
2:M:207:THR:OG1	2:M:210:GLU:HG2	1.92	0.68
1:A:168:ASP:OD1	1:A:172:ASN:N	2.26	0.68
2:I:339:ARG:HG2	2:I:842:ASN:HD22	1.57	0.68
2:B:865:ASN:O	2:B:867:GLU:N	2.28	0.68
3:J:110:PRO:HG2	3:J:146:ASP:HA	1.75	0.68
2:M:56:ARG:NH2	2:M:136:ASP:OD1	2.27	0.68
3:N:85:PHE:CA	3:N:96:LYS:HE3	2.24	0.67
2:B:177:ILE:HB	2:B:984:PHE:HB2	1.75	0.67
2:I:207:THR:OG1	2:I:210:GLU:HG2	1.94	0.67
2:I:328:LEU:HD22	2:I:366:MET:HE2	1.77	0.67
1:A:138:TRP:NE1	1:A:465:THR:HG22	2.09	0.67
1:A:333:TYR:CD2	1:A:342:ASN:HB3	2.30	0.67
2:B:505:LEU:HD12	2:I:516:GLN:HB3	1.76	0.67
1:H:229:GLU:O	1:H:233:ARG:NH1	2.27	0.67
2:I:56:ARG:HD2	2:I:979:ASN:ND2	2.10	0.67
1:A:265:ARG:HG2	1:A:358:ARG:HD2	1.77	0.67
2:I:107:VAL:HG11	2:I:405:GLY:HA3	1.76	0.67
2:B:56:ARG:O	2:B:254:ARG:NH2	2.22	0.67
2:D:893:ASP:HB2	2:D:897:CYS:HB2	1.77	0.67
1:H:38:ILE:HG22	1:H:401:MET:HG3	1.77	0.67
1:H:272:LYS:HG3	1:H:279:TYR:CE1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:186:SER:HB2	2:M:252:GLY:HA3	1.77	0.67
2:M:923:LYS:HZ3	2:M:924:THR:HG23	1.59	0.67
1:C:68:GLU:OE2	1:C:459:ARG:NH1	2.28	0.66
3:F:23:VAL:HG13	3:F:135:VAL:HG12	1.78	0.66
1:H:188:ARG:NE	1:H:402:GLU:OE2	2.28	0.66
2:I:402:TYR:OH	2:I:459:GLN:NE2	2.29	0.66
2:B:447:TYR:CD1	2:B:503:PHE:HB3	2.30	0.66
2:D:419:ASN:ND2	2:D:422:ALA:HB3	2.09	0.66
1:H:124:TYR:O	1:H:125:SER:HB3	1.94	0.66
2:M:333:SER:OG	2:M:366:MET:O	2.08	0.66
1:A:333:TYR:HD2	1:A:342:ASN:HB3	1.60	0.65
2:B:583:THR:HG21	2:B:658:LYS:HA	1.78	0.65
3:J:46:TYR:OH	3:J:68:LYS:NZ	2.29	0.65
2:B:833:THR:OG1	2:B:966:GLU:OE2	2.14	0.65
2:B:845:GLN:HE22	2:B:947:THR:HG21	1.59	0.65
2:D:611:SER:HB2	2:D:620:THR:HG22	1.79	0.65
2:D:981:MET:HE1	2:D:983:LYS:HB2	1.77	0.65
1:L:209:THR:C	1:L:212:GLN:HG2	2.16	0.65
2:B:527:PHE:HB3	2:B:545:ARG:HD2	1.78	0.65
2:D:511:THR:HG23	2:M:511:THR:HG23	1.78	0.65
2:D:722:TRP:HD1	2:D:806:VAL:HG12	1.61	0.65
3:N:86:VAL:H	3:N:96:LYS:CE	2.10	0.65
2:M:288:ASP:OD1	2:M:288:ASP:N	2.28	0.64
2:I:832:ARG:HG2	2:I:968:THR:HG23	1.79	0.64
1:L:416:SER:HB2	1:L:434:GLU:HG3	1.79	0.64
3:N:12:VAL:HA	3:N:75:TYR:CE2	2.32	0.64
2:B:774:GLN:HE22	2:B:776:ARG:HG3	1.62	0.64
1:H:427:GLU:OE1	1:H:427:GLU:N	2.27	0.64
2:M:242:PRO:HA	2:M:339:ARG:HH12	1.62	0.64
1:C:271:SER:O	1:C:305:SER:HB2	1.97	0.64
2:D:579:GLN:HA	2:D:580:ASP:CB	2.27	0.64
1:H:286:GLY:H	1:H:287:LYS:HZ3	1.46	0.64
2:I:575:ASN:HB2	2:I:577:ASN:HB2	1.80	0.64
1:L:205:GLU:O	1:L:209:THR:HG22	1.98	0.64
2:M:714:LYS:O	2:M:714:LYS:HD3	1.97	0.64
1:A:27:SER:HB3	1:A:170:ILE:HD11	1.80	0.63
2:B:753:MET:HE3	2:B:964:TYR:HA	1.77	0.63
2:D:502:TRP:HB3	2:D:507:ASN:HD22	1.63	0.63
2:I:658:LYS:HD3	2:I:660:ARG:HG3	1.79	0.63
2:B:200:MET:HE1	2:B:225:TRP:HB2	1.79	0.63
1:A:263:ASP:OD2	1:A:265:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:406:GLU:OE1	1:H:409:ARG:NH1	2.32	0.63
3:N:86:VAL:H	3:N:96:LYS:HE3	1.63	0.63
3:N:116:ASP:OD2	3:N:139:ARG:NH1	2.31	0.63
1:C:282:GLN:NE2	1:C:299:TRP:HE1	1.95	0.63
2:M:169:GLY:HA2	2:M:262:ASN:OD1	1.97	0.63
3:N:86:VAL:H	3:N:96:LYS:NZ	1.97	0.63
2:B:105:ASP:H	2:B:107:VAL:H	1.45	0.63
1:L:272:LYS:HD3	1:L:279:TYR:HE1	1.64	0.63
2:B:207:THR:HB	2:B:210:GLU:HG2	1.81	0.62
1:C:296:THR:CG2	2:D:205:ASN:HD22	2.12	0.62
1:L:354:ASP:OD2	1:L:394:SER:HA	1.99	0.62
1:L:449:MET:HE3	1:L:451:ARG:H	1.62	0.62
2:B:785:LEU:HD23	2:B:878:ILE:HG12	1.82	0.62
1:A:255:VAL:HG11	1:A:281:GLY:HA3	1.80	0.62
2:B:332:ASN:OD1	2:B:832:ARG:NH2	2.32	0.62
2:D:741:ILE:HG13	2:D:756:ILE:HG12	1.79	0.62
1:L:354:ASP:OD1	1:L:358:ARG:NE	2.24	0.62
2:M:489:TYR:OH	2:M:515:GLU:OE2	2.13	0.62
1:C:137:LYS:NZ	1:C:139:ASP:OD1	2.33	0.62
1:H:213:ASN:HB3	1:H:215:GLU:HG3	1.80	0.62
2:I:65:ALA:HB3	2:I:908:ARG:HD3	1.82	0.62
1:L:414:LYS:HD2	1:L:415:LEU:H	1.63	0.62
3:N:23:VAL:HG11	3:N:64:PHE:CZ	2.34	0.62
1:A:257:TYR:HE2	1:A:389:MET:HB3	1.65	0.62
2:D:833:THR:OG1	2:D:966:GLU:OE2	2.16	0.62
2:D:430:ASN:N	2:D:431:GLY:HA3	2.15	0.62
1:L:229:GLU:O	1:L:233:ARG:CZ	2.48	0.62
1:L:407:ILE:HG12	1:L:413:PRO:HD2	1.81	0.62
3:J:82:THR:OG1	3:J:97:ILE:N	2.30	0.61
2:B:51:LYS:HA	2:B:54:GLU:OE1	1.99	0.61
1:H:119:THR:HG23	1:H:454:TYR:CE1	2.35	0.61
2:B:640:LEU:HD22	2:B:676:ILE:HD13	1.83	0.61
2:D:598:ALA:HB2	2:D:676:ILE:HD12	1.82	0.61
3:E:23:VAL:HG11	3:E:64:PHE:CZ	2.35	0.61
1:H:205:GLU:O	1:H:209:THR:HG23	2.00	0.61
2:B:430:ASN:N	2:B:431:GLY:HA3	2.16	0.61
1:H:418:TYR:CD2	1:H:429:VAL:HG22	2.36	0.61
2:B:224:LEU:HD23	2:B:235:LEU:HD13	1.83	0.61
1:L:204:THR:O	1:L:208:LYS:HG3	2.00	0.61
1:H:119:THR:HG21	1:H:138:TRP:HZ3	1.66	0.60
2:M:244:ASN:OD1	2:M:339:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:PRO:HG3	3:F:46:TYR:CZ	2.37	0.60
1:C:371:ALA:O	1:C:373:ALA:N	2.32	0.60
1:L:123:PRO:HD3	1:L:138:TRP:CD2	2.36	0.60
2:B:68:ILE:HB	2:B:71:VAL:CG2	2.32	0.60
1:L:175:ILE:O	1:L:179:LYS:HG3	2.02	0.60
1:C:136:PRO:HD2	1:C:462:ASN:ND2	2.17	0.60
2:D:333:SER:HG	2:D:366:MET:H	1.48	0.60
1:H:34:VAL:O	1:H:39:TYR:HB2	2.01	0.60
2:I:306:LEU:HD11	2:I:390:LEU:HD11	1.82	0.60
3:N:58:LEU:H	3:N:68:LYS:NZ	1.99	0.60
1:C:92:LEU:O	1:C:101:ARG:NH1	2.34	0.60
2:I:404:MET:SD	2:I:459:GLN:NE2	2.75	0.60
2:I:430:ASN:N	2:I:431:GLY:HA3	2.17	0.60
2:I:105:ASP:O	2:I:387:LYS:NZ	2.34	0.60
2:I:730:LYS:HG2	2:I:732:ILE:HD13	1.82	0.60
1:A:352:THR:HA	1:A:364:GLU:HG2	1.83	0.60
1:L:391:LYS:O	1:L:395:LEU:HD12	2.01	0.60
2:I:473:ASN:HB3	2:I:533:SER:HB3	1.82	0.59
2:M:813:LYS:CG	2:M:814:GLY:H	2.14	0.59
1:L:418:TYR:HE2	1:L:429:VAL:HG12	1.67	0.59
3:N:65:TRP:HE1	3:N:91:TYR:HH	1.45	0.59
1:C:340:ASP:OD2	1:C:383:LYS:NZ	2.34	0.59
2:M:813:LYS:HG3	2:M:814:GLY:H	1.67	0.59
2:I:95:SER:HB2	2:I:677:PHE:HE1	1.67	0.59
1:H:191:LEU:HD13	1:H:328:LEU:HD23	1.85	0.59
2:I:571:SER:OG	2:I:585:GLY:N	2.36	0.59
3:E:21:VAL:HG12	3:E:137:GLY:HA3	1.84	0.59
1:H:459:ARG:NH2	1:H:466:PRO:O	2.35	0.59
2:B:138:VAL:HG22	2:B:164:ILE:HD11	1.83	0.59
3:J:21:VAL:HG21	3:J:43:MET:HE2	1.85	0.59
1:L:232:LYS:NZ	2:M:620:THR:O	2.35	0.59
2:M:430:ASN:N	2:M:431:GLY:HA3	2.17	0.59
1:H:255:VAL:HG11	1:H:281:GLY:HA3	1.84	0.59
2:I:317:GLN:HG2	2:I:381:SER:HB3	1.83	0.59
1:A:263:ASP:OD1	1:A:265:ARG:HD3	2.01	0.59
2:D:785:LEU:HD23	2:D:878:ILE:CD1	2.32	0.59
1:H:354:ASP:OD2	1:H:394:SER:HA	2.02	0.59
2:I:200:MET:HE1	2:I:225:TRP:HB2	1.83	0.59
3:N:12:VAL:HA	3:N:75:TYR:HE2	1.68	0.59
2:D:938:LEU:O	2:D:974:ARG:NH1	2.35	0.58
1:A:100:ASP:O	1:A:104:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:893:ASP:HB2	2:I:897:CYS:HB2	1.85	0.58
2:B:774:GLN:HE21	2:B:776:ARG:HE	1.50	0.58
2:I:837:ASN:HA	2:I:840:THR:HG22	1.86	0.58
2:B:834:LYS:NZ	2:B:897:CYS:O	2.36	0.58
2:M:105:ASP:O	2:M:387:LYS:NZ	2.30	0.58
2:M:195:GLN:HG2	2:M:197:GLU:H	1.67	0.58
1:L:266:ILE:HG13	1:L:279:TYR:CD2	2.39	0.58
2:I:389:GLN:NE2	2:I:391:ASP:OD1	2.36	0.58
2:B:516:GLN:HB2	2:I:505:LEU:HD12	1.86	0.58
2:B:853:PRO:HD2	3:F:17:GLY:HA2	1.84	0.58
1:H:171:PHE:HZ	1:H:221:VAL:HG22	1.68	0.58
1:A:50:GLU:HG3	1:A:282:GLN:HE21	1.69	0.57
2:B:40:LEU:HD21	2:B:42:TYR:CZ	2.39	0.57
2:D:447:TYR:CD1	2:D:503:PHE:HB3	2.38	0.57
1:L:171:PHE:CE1	1:L:177:GLN:HG2	2.39	0.57
1:L:255:VAL:HG11	1:L:281:GLY:N	2.19	0.57
1:A:2:ASP:O	2:B:522:ARG:NH1	2.34	0.57
1:A:68:GLU:OE1	1:A:459:ARG:HD2	2.04	0.57
3:E:116:ASP:OD2	3:E:139:ARG:NH2	2.32	0.57
2:I:596:ASN:HB3	2:I:643:GLU:HB3	1.86	0.57
1:L:339:ASP:CG	1:L:342:ASN:HB2	2.24	0.57
3:N:24:ASN:HA	3:N:33:GLU:O	2.04	0.57
1:L:426:SER:O	1:L:429:VAL:HG23	2.03	0.57
1:H:141:GLY:HA3	1:H:476:TRP:CD1	2.39	0.57
1:H:348:GLU:HB3	1:H:368:LEU:HD22	1.85	0.57
2:I:822:ASP:OD2	2:I:908:ARG:NH1	2.37	0.57
2:B:588:ARG:NH2	2:B:664:ASP:OD2	2.37	0.57
1:C:68:GLU:OE1	1:C:459:ARG:HD2	2.04	0.57
2:D:579:GLN:HG3	2:D:581:VAL:N	2.19	0.57
2:B:58:SER:HB2	2:B:277:ILE:HD13	1.86	0.57
2:I:598:ALA:HB2	2:I:676:ILE:HD13	1.86	0.57
3:J:26:PHE:HA	3:J:30:LYS:O	2.05	0.57
2:M:195:GLN:NE2	2:M:841:GLY:O	2.36	0.57
2:M:937:ASN:ND2	2:M:973:SER:O	2.38	0.57
1:A:194:ILE:HG13	1:A:195:ASP:N	2.19	0.57
1:H:444:GLU:OE2	2:I:862:LYS:NZ	2.37	0.57
2:I:756:ILE:HB	2:I:759:MET:HG3	1.87	0.57
3:N:16:ALA:O	3:N:139:ARG:NH2	2.37	0.57
1:A:449:MET:HE3	1:A:471:GLY:HA3	1.86	0.57
2:B:430:ASN:O	2:B:439:PRO:HD2	2.05	0.57
2:B:579:GLN:HB2	2:B:581:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:419:ASN:HD21	2:D:422:ALA:CB	2.16	0.57
3:F:120:TYR:CZ	3:F:135:VAL:HG21	2.39	0.57
1:H:187:LEU:O	1:H:191:LEU:HD12	2.05	0.57
1:L:392:TRP:CD1	1:L:407:ILE:HD11	2.40	0.57
2:B:195:GLN:HG2	2:B:197:GLU:H	1.69	0.57
1:C:119:THR:O	1:C:121:ASP:N	2.38	0.57
1:H:324:GLU:O	1:H:328:LEU:HD12	2.05	0.57
2:I:549:SER:O	2:I:557:ARG:HD3	2.05	0.57
1:L:212:GLN:HG3	1:L:213:ASN:N	2.19	0.57
2:B:53:ALA:O	2:B:56:ARG:HD2	2.05	0.56
2:M:236:LYS:NZ	2:M:340:ASP:OD2	2.35	0.56
1:C:124:TYR:C	1:C:126:GLU:H	2.08	0.56
2:I:267:LYS:HZ3	2:I:302:LYS:H	1.54	0.56
3:E:92:GLU:O	3:E:92:GLU:HG3	2.05	0.56
2:B:40:LEU:HD11	2:B:42:TYR:CE2	2.40	0.56
2:D:338:PRO:HB2	2:D:341:ILE:HG12	1.86	0.56
2:B:722:TRP:HD1	2:B:806:VAL:HG12	1.71	0.56
1:L:27:SER:HB3	1:L:170:ILE:HD11	1.88	0.56
2:M:406:LEU:HD13	2:M:457:ILE:HD11	1.87	0.56
2:B:657:PHE:O	2:B:658:LYS:HB2	2.06	0.56
1:H:427:GLU:OE2	1:H:428:SER:OG	2.23	0.56
1:H:449:MET:HE1	1:H:451:ARG:O	2.05	0.56
2:B:104:VAL:HA	2:B:164:ILE:CG2	2.35	0.56
2:B:394:PHE:HD2	2:B:395:LEU:HG	1.71	0.56
2:M:611:SER:HB2	2:M:620:THR:HG22	1.87	0.56
1:A:24:PRO:HB3	1:A:169:LEU:HD11	1.87	0.56
2:B:788:GLU:HA	2:B:894:MET:HE2	1.87	0.56
1:A:119:THR:O	1:A:121:ASP:N	2.39	0.56
2:B:57:THR:OG1	2:B:59:ASP:O	2.24	0.56
2:I:959:ASP:OD1	2:I:960:LEU:N	2.38	0.56
2:M:581:VAL:HG13	2:M:657:PHE:CE1	2.41	0.56
2:D:545:ARG:NE	2:D:547:ASP:OD1	2.36	0.55
2:I:829:MET:HE2	2:I:902:LYS:HA	1.88	0.55
2:B:671:ASN:HD22	2:B:696:LYS:HD3	1.70	0.55
2:B:774:GLN:NE2	2:B:776:ARG:HE	2.04	0.55
1:H:159:LEU:HD13	1:H:175:ILE:HD11	1.88	0.55
2:M:56:ARG:HD2	2:M:979:ASN:CG	2.27	0.55
2:D:177:ILE:HB	2:D:984:PHE:HB2	1.88	0.55
2:D:200:MET:HE1	2:D:225:TRP:HB2	1.88	0.55
2:I:845:GLN:HE22	2:I:947:THR:HG21	1.71	0.55
1:L:266:ILE:HG13	1:L:279:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:CE2	1:A:104:THR:HG22	2.41	0.55
3:F:11:ALA:HB1	3:F:53:GLU:HG3	1.87	0.55
1:C:195:ASP:OD1	1:C:335:ARG:NH2	2.28	0.55
2:I:652:LEU:HD11	2:I:654:MET:HE2	1.89	0.55
1:H:286:GLY:N	1:H:287:LYS:HZ3	2.04	0.55
1:H:331:GLU:CD	1:H:409:ARG:HH22	2.09	0.55
1:H:347:TYR:CD1	1:H:387:ILE:HG22	2.41	0.55
2:I:282:MET:SD	2:I:973:SER:HB3	2.46	0.55
2:I:430:ASN:O	2:I:439:PRO:HD2	2.07	0.55
1:H:119:THR:HG22	1:H:121:ASP:O	2.06	0.55
2:I:169:GLY:HA2	2:I:262:ASN:OD1	2.07	0.55
2:I:242:PRO:HA	2:I:339:ARG:HH22	1.72	0.55
1:L:142:GLU:HA	1:L:145:TYR:HB2	1.89	0.55
1:L:272:LYS:HD3	1:L:279:TYR:CE1	2.42	0.55
1:A:141:GLY:HA3	1:A:476:TRP:CD1	2.42	0.55
1:C:34:VAL:O	1:C:39:TYR:HB2	2.07	0.54
2:I:447:TYR:CD1	2:I:503:PHE:HB3	2.41	0.54
2:M:124:TYR:OH	2:M:415:LYS:NZ	2.25	0.54
1:A:34:VAL:O	1:A:39:TYR:HB2	2.06	0.54
1:A:379:THR:O	1:A:383:LYS:HD3	2.08	0.54
2:B:665:VAL:HG12	2:B:704:LEU:HD23	1.89	0.54
1:L:321:THR:HG22	1:L:324:GLU:H	1.73	0.54
2:M:823:ILE:HG12	2:M:905:VAL:HG22	1.89	0.54
2:B:906:LYS:HD3	2:B:937:ASN:OD1	2.07	0.54
2:I:938:LEU:HA	2:I:974:ARG:HG3	1.89	0.54
2:B:645:THR:HG22	2:B:672:THR:HG23	1.89	0.54
2:D:38:LYS:O	2:D:586:LYS:NZ	2.40	0.54
2:D:281:GLY:H	2:D:288:ASP:HB2	1.73	0.54
1:L:87:ASP:O	1:L:91:VAL:HG23	2.07	0.54
1:A:220:ASP:HB2	1:A:222:LYS:HD2	1.89	0.54
2:D:218:PHE:CE2	2:D:240:ALA:HB2	2.43	0.54
2:D:579:GLN:NE2	2:D:580:ASP:HB3	2.21	0.54
1:A:430:TYR:CE2	1:A:432:PRO:HA	2.43	0.54
2:D:967:TYR:O	2:D:968:THR:OG1	2.20	0.54
1:L:120:SER:HB2	1:L:475:VAL:HG12	1.89	0.54
2:B:569:ILE:HD12	2:B:585:GLY:O	2.08	0.54
2:D:502:TRP:HB3	2:D:507:ASN:ND2	2.23	0.54
2:B:195:GLN:NE2	2:B:198:PHE:O	2.34	0.54
1:H:85:LEU:HB3	1:H:128:LEU:HD11	1.90	0.54
2:M:421:TYR:HD1	2:M:421:TYR:O	1.91	0.54
2:M:834:LYS:NZ	2:M:897:CYS:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:TYR:O	1:C:126:GLU:N	2.40	0.54
3:F:85:PHE:HB3	3:F:94:LYS:HG2	1.90	0.54
2:M:289:SER:HB2	2:M:320:ASN:HB2	1.90	0.54
1:A:257:TYR:HE1	1:A:261:THR:HG21	1.73	0.53
3:N:96:LYS:O	3:N:122:VAL:HA	2.07	0.53
1:A:451:ARG:HD2	1:A:473:THR:O	2.09	0.53
2:B:587:ILE:HD11	2:B:652:LEU:HD12	1.89	0.53
2:B:40:LEU:HD12	2:B:41:GLY:H	1.74	0.53
2:B:453:ARG:NH2	2:I:380:GLU:OE1	2.40	0.53
1:H:255:VAL:HG11	1:H:281:GLY:CA	2.38	0.53
1:L:54:GLU:HB2	1:L:301:ASN:OD1	2.09	0.53
1:A:138:TRP:CE2	1:A:465:THR:HG22	2.43	0.53
1:H:272:LYS:HG3	1:H:279:TYR:HE1	1.71	0.53
2:M:218:PHE:HE1	2:M:340:ASP:HB3	1.74	0.53
1:A:352:THR:HG22	1:A:364:GLU:HG2	1.90	0.53
1:L:34:VAL:O	1:L:39:TYR:HB2	2.09	0.53
2:D:762:GLY:HA3	2:D:798:MET:HG2	1.89	0.53
1:H:248:HIS:ND1	1:H:309:TYR:OH	2.40	0.53
1:A:458:ALA:HB1	1:A:465:THR:HG21	1.89	0.53
2:D:302:LYS:HE2	2:D:304:GLY:O	2.08	0.53
2:D:328:LEU:HD22	2:D:366:MET:HE2	1.91	0.53
1:H:407:ILE:HG12	1:H:413:PRO:HD2	1.89	0.53
2:I:267:LYS:NZ	2:I:302:LYS:H	2.05	0.53
2:B:919:ARG:O	2:B:921:LEU:N	2.41	0.53
1:C:229:GLU:O	1:C:233:ARG:NH2	2.42	0.53
2:I:419:ASN:ND2	2:I:444:THR:O	2.42	0.53
2:I:845:GLN:HE22	2:I:947:THR:CG2	2.22	0.53
1:L:27:SER:CB	1:L:170:ILE:HD11	2.39	0.53
3:N:67:TYR:CD2	3:N:95:VAL:HG11	2.44	0.53
3:N:85:PHE:HA	3:N:96:LYS:CD	2.38	0.53
2:B:475:ASN:HB3	2:B:531:GLU:HB3	1.89	0.52
2:B:675:GLN:HE22	2:B:697:ILE:HD13	1.74	0.52
3:F:110:PRO:HG2	3:F:146:ASP:HA	1.89	0.52
2:M:105:ASP:H	2:M:107:VAL:H	1.58	0.52
2:M:430:ASN:O	2:M:439:PRO:HD2	2.08	0.52
2:M:511:THR:HG22	2:M:512:PRO:O	2.10	0.52
3:N:71:VAL:CG1	3:N:80:PHE:HB2	2.38	0.52
3:N:85:PHE:CD2	3:N:96:LYS:HG2	2.45	0.52
3:N:86:VAL:HG12	3:N:87:ASP:H	1.75	0.52
1:C:204:THR:O	1:C:207:VAL:HG12	2.10	0.52
2:B:104:VAL:HA	2:B:164:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:LEU:HD22	2:B:366:MET:HE2	1.90	0.52
2:D:773:PRO:HD2	2:D:871:TYR:CE1	2.45	0.52
1:C:53:PRO:HD2	1:C:301:ASN:HD22	1.75	0.52
1:C:97:ASN:ND2	1:C:165[B]:ASP:OD1	2.42	0.52
1:L:418:TYR:CE2	1:L:429:VAL:HG12	2.44	0.52
2:M:111:ASN:HA	2:M:129:GLY:HA3	1.91	0.52
1:H:43:GLY:HA3	1:H:49:TYR:CZ	2.45	0.52
1:H:251:ALA:O	1:H:255:VAL:HG12	2.10	0.52
2:D:545:ARG:HG2	2:D:561:TYR:CZ	2.45	0.52
1:L:102:PHE:CZ	1:L:106:ILE:HD11	2.45	0.52
3:N:97:ILE:HA	3:N:121:MET:O	2.10	0.52
2:D:579:GLN:CD	2:D:580:ASP:HB3	2.31	0.52
2:D:715:ASP:O	2:D:812:TYR:HA	2.09	0.52
2:I:224:LEU:HD23	2:I:235:LEU:HD13	1.92	0.52
1:L:253:PRO:HA	1:L:430:TYR:OH	2.09	0.52
2:M:938:LEU:O	2:M:974:ARG:NH1	2.42	0.52
2:D:523:LEU:HD21	2:D:547:ASP:HB3	1.92	0.52
1:L:476:TRP:CE2	1:L:477:TRP:HD1	2.27	0.52
2:B:713:THR:HG22	2:B:715:ASP:N	2.25	0.51
1:L:85:LEU:HB3	1:L:128:LEU:HD11	1.92	0.51
3:F:27:ILE:HG12	3:F:131:LEU:HD21	1.91	0.51
2:I:767:GLN:HG2	2:I:895:GLY:N	2.23	0.51
2:M:635:LEU:HD23	2:M:636:GLY:O	2.10	0.51
2:M:731:VAL:HG23	2:M:761:VAL:HG12	1.92	0.51
2:B:314:TYR:OH	2:I:455:ARG:NH1	2.43	0.51
2:D:169:GLY:HA2	2:D:262:ASN:HB2	1.92	0.51
1:L:123:PRO:HD3	1:L:138:TRP:CE2	2.45	0.51
2:I:788:GLU:HA	2:I:894:MET:CE	2.41	0.51
2:B:419:ASN:HB3	2:B:500:PRO:HB3	1.92	0.51
2:B:665:VAL:CG1	2:B:704:LEU:HD23	2.41	0.51
2:D:863:ILE:HB	2:D:870:THR:HG23	1.92	0.51
2:I:419:ASN:O	2:I:423:LEU:HD12	2.11	0.51
2:I:836:ILE:O	2:I:840:THR:HG22	2.10	0.51
2:B:169:GLY:HA3	2:B:269:ASP:HB2	1.92	0.51
2:B:410:THR:HA	2:B:452:THR:O	2.11	0.51
1:H:191:LEU:HD22	1:H:409:ARG:NH2	2.26	0.51
2:B:64:LEU:HD11	2:B:141:MET:CE	2.41	0.51
3:E:13:GLU:HG2	3:E:14:LYS:HG2	1.93	0.51
1:H:229:GLU:O	1:H:233:ARG:CZ	2.59	0.51
2:I:59:ASP:OD2	2:I:62:SER:N	2.40	0.51
2:I:753:MET:HE1	2:I:764:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HD2	1:A:384:LEU:HD21	1.92	0.51
2:D:579:GLN:HG3	2:D:581:VAL:H	1.74	0.51
3:F:21:VAL:HG21	3:F:43:MET:HE2	1.91	0.51
1:H:418:TYR:CE2	1:H:429:VAL:HG22	2.45	0.51
2:I:331:LEU:HD22	2:I:970:ASN:HA	1.92	0.51
2:I:489:TYR:OH	2:I:515:GLU:OE2	2.20	0.51
1:L:219:GLY:O	1:L:322:GLN:HB2	2.10	0.51
2:M:767:GLN:CG	2:M:895:GLY:H	2.24	0.51
3:N:86:VAL:N	3:N:96:LYS:HE3	2.25	0.51
1:H:412:CYS:HA	1:H:413:PRO:C	2.31	0.51
2:M:447:TYR:CD1	2:M:503:PHE:HB3	2.46	0.51
1:A:207:VAL:O	1:A:211:VAL:HG23	2.11	0.51
2:I:73:ILE:HG12	2:I:86:VAL:HG22	1.92	0.51
1:L:258:LEU:HB2	1:L:266:ILE:HD13	1.93	0.51
1:L:391:LYS:NZ	1:L:406:GLU:OE1	2.37	0.51
2:M:197:GLU:OE2	2:M:217:ARG:NH1	2.43	0.51
1:A:156:GLU:OE1	1:A:186:ARG:NH2	2.44	0.50
1:H:183:ASN:HA	1:H:186:ARG:HD2	1.93	0.50
1:C:459:ARG:NH2	1:C:465:THR:O	2.44	0.50
2:D:579:GLN:HG3	2:D:581:VAL:HB	1.93	0.50
1:L:201:ALA:O	1:L:205:GLU:HG2	2.11	0.50
2:B:856:VAL:O	2:B:859:SER:OG	2.19	0.50
1:C:126:GLU:O	1:C:136:PRO:HB3	2.11	0.50
2:D:97:THR:O	2:D:97:THR:OG1	2.24	0.50
3:F:75:TYR:O	3:F:78:ARG:NH1	2.44	0.50
1:H:255:VAL:HG11	1:H:281:GLY:N	2.27	0.50
1:L:333:TYR:CD2	1:L:342:ASN:HB3	2.46	0.50
1:A:251:ALA:O	1:A:255:VAL:HG12	2.11	0.50
2:B:138:VAL:CG2	2:B:164:ILE:HD11	2.41	0.50
2:D:938:LEU:HA	2:D:974:ARG:HG3	1.92	0.50
1:L:148:ILE:HA	1:L:151:GLU:HG3	1.93	0.50
1:L:324:GLU:O	1:L:328:LEU:HD12	2.10	0.50
3:N:58:LEU:HD11	3:N:120:TYR:CE2	2.45	0.50
1:A:257:TYR:CE2	1:A:389:MET:HB3	2.44	0.50
2:B:498:THR:HG21	2:I:627:ASN:HD22	1.77	0.50
2:B:657:PHE:HB2	2:B:660:ARG:HB2	1.93	0.50
2:I:772:ASP:OD2	2:I:776:ARG:HB2	2.10	0.50
1:A:97:ASN:O	1:A:101:ARG:HG3	2.11	0.50
2:B:97:THR:O	2:B:97:THR:OG1	2.26	0.50
2:D:767:GLN:HG2	2:D:895:GLY:N	2.24	0.50
2:B:473:ASN:HB3	2:B:533:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:LEU:HD11	2:B:722:TRP:CZ3	2.47	0.50
1:C:57:GLN:HG2	1:C:244:LEU:HD13	1.93	0.50
1:C:191:LEU:HD13	1:C:409:ARG:HH12	1.77	0.50
2:D:407:ASP:O	2:D:455:ARG:HA	2.12	0.50
1:A:114:ILE:O	1:A:118:ASN:ND2	2.43	0.50
1:A:229:GLU:O	1:A:233:ARG:NH2	2.45	0.50
2:D:523:LEU:HD22	2:D:548:TRP:O	2.11	0.50
2:D:829:MET:HE1	2:D:902:LYS:HA	1.94	0.50
3:F:13:GLU:HG3	3:F:14:LYS:N	2.27	0.50
3:J:15:MET:HE1	3:J:75:TYR:HA	1.92	0.50
2:M:244:ASN:OD1	2:M:245:ILE:N	2.44	0.50
3:N:23:VAL:HG22	3:N:135:VAL:HG12	1.93	0.50
2:B:194:PHE:CZ	2:B:245:ILE:HD12	2.47	0.50
2:D:198:PHE:CZ	2:D:851:ARG:HD2	2.47	0.50
1:L:266:ILE:HG23	1:L:279:TYR:CE2	2.47	0.50
1:L:430:TYR:CE2	1:L:432:PRO:HA	2.47	0.50
2:M:37:GLU:HG3	2:M:38:LYS:H	1.77	0.50
2:M:669:ASN:OD1	2:M:700:ARG:HD3	2.12	0.50
1:A:190:TYR:HB3	1:A:207:VAL:HG23	1.94	0.49
1:A:333:TYR:CD1	1:A:337:HIS:CD2	3.00	0.49
3:F:129:ASP:HB3	3:F:131:LEU:HD13	1.94	0.49
2:B:661:LEU:HD12	2:B:708:GLY:HA3	1.94	0.49
1:C:275:ALA:HB2	1:C:302:LYS:HG2	1.94	0.49
1:H:145:TYR:CE2	1:H:189:MET:HG2	2.47	0.49
2:I:452:THR:HG23	2:I:489:TYR:HB3	1.94	0.49
2:D:536:ASN:HA	2:D:539:TYR:OH	2.12	0.49
1:H:277:GLY:O	1:H:278:LYS:HG2	2.12	0.49
2:I:576:ASP:HA	2:I:579:GLN:HB3	1.94	0.49
3:N:120:TYR:CZ	3:N:135:VAL:HG21	2.47	0.49
3:E:93:SER:OG	3:E:94:LYS:N	2.45	0.49
1:L:34:VAL:HG11	1:L:114:ILE:CD1	2.37	0.49
1:L:416:SER:C	1:L:418:TYR:H	2.15	0.49
3:N:41:LEU:HD23	3:N:63:ASN:HB3	1.94	0.49
1:A:123:PRO:HD3	1:A:138:TRP:CD2	2.48	0.49
1:C:75:TYR:CD2	2:D:615:PRO:HD3	2.48	0.49
3:E:113:MET:HG3	3:E:114:PRO:HD2	1.94	0.49
1:H:321:THR:HG23	1:H:324:GLU:H	1.77	0.49
1:L:183:ASN:OD1	1:L:186:ARG:NH1	2.46	0.49
2:B:834:LYS:HD3	2:B:898:PHE:HD1	1.76	0.49
2:D:454:ARG:HG2	2:D:487:VAL:HG23	1.94	0.49
2:I:760:PRO:HG2	2:I:797:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:771:ARG:NH1	2:I:777:ILE:HB	2.28	0.49
1:L:54:GLU:OE2	1:L:300:LYS:HB3	2.12	0.49
1:L:81:PHE:HE2	1:L:115:MET:HG2	1.76	0.49
2:D:456:GLU:HG3	2:D:485:ARG:HG2	1.95	0.49
1:H:266:ILE:HG12	1:H:279:TYR:CD2	2.47	0.49
2:B:295:PHE:HE2	2:I:312:LEU:HD21	1.77	0.49
1:H:38:ILE:CG2	1:H:401:MET:HG3	2.42	0.49
2:I:302:LYS:HB2	2:I:307:THR:HG23	1.93	0.49
2:B:356:PRO:HG2	2:B:424:TYR:CZ	2.47	0.49
1:C:37:GLU:HG2	1:C:76:SER:OG	2.12	0.49
2:D:596:ASN:HB3	2:D:643:GLU:HB3	1.94	0.49
2:I:188:VAL:CG2	2:I:282:MET:HE1	2.43	0.49
3:J:93:SER:OG	3:J:94:LYS:N	2.45	0.49
1:L:89:LYS:O	1:L:93:GLU:HG3	2.12	0.49
1:A:171:PHE:HZ	1:A:221:VAL:HG22	1.78	0.49
2:D:362:PRO:HB3	2:D:430:ASN:OD1	2.12	0.49
1:H:476:TRP:CZ3	1:H:477:TRP:HB3	2.47	0.49
1:L:255:VAL:HG11	1:L:281:GLY:HA3	1.94	0.49
1:A:164:MET:CE	1:A:173:LYS:HA	2.42	0.48
1:A:335:ARG:HG3	1:A:384:LEU:HD11	1.95	0.48
2:B:583:THR:OG1	2:B:658:LYS:N	2.36	0.48
2:B:690:GLN:HG2	2:B:692:MET:HG3	1.94	0.48
1:L:171:PHE:CD1	1:L:177:GLN:HG2	2.48	0.48
1:A:85:LEU:HB3	1:A:128:LEU:HD11	1.95	0.48
1:A:219:GLY:O	1:A:322:GLN:HB2	2.13	0.48
1:A:252:TYR:OH	1:A:427:GLU:OE1	2.24	0.48
1:L:194:ILE:HD11	1:L:204:THR:N	2.28	0.48
1:L:257:TYR:CZ	1:L:389:MET:HE2	2.47	0.48
2:B:200:MET:HG3	2:B:210:GLU:HB2	1.94	0.48
2:D:184:GLN:HG2	2:D:254:ARG:HB3	1.95	0.48
2:D:190:ARG:HH22	2:D:942:THR:HG22	1.78	0.48
2:M:527:PHE:HB3	2:M:545:ARG:HD2	1.96	0.48
2:M:668:TYR:CZ	2:M:701:GLY:HA3	2.48	0.48
2:B:94:LEU:HD12	2:B:94:LEU:HA	1.63	0.48
2:B:516:GLN:NE2	2:I:447:TYR:OH	2.44	0.48
2:D:190:ARG:HH12	2:D:942:THR:CG2	2.21	0.48
2:I:101:LEU:HD11	2:I:108:PRO:HB3	1.95	0.48
2:I:166:THR:HB	2:I:298:ARG:NH1	2.29	0.48
2:I:326:GLN:NE2	4:K:5:GLY:HA2	2.24	0.48
2:I:588:ARG:NH2	2:I:664:ASP:OD1	2.44	0.48
2:M:195:GLN:HG3	2:M:847:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:419:ASN:ND2	2:M:444:THR:O	2.47	0.48
2:B:99:GLN:NE2	2:B:959:ASP:OD1	2.43	0.48
2:B:761:VAL:O	2:B:798:MET:HE2	2.14	0.48
3:E:85:PHE:O	3:E:94:LYS:NZ	2.47	0.48
1:H:268:TYR:CZ	1:H:311:ILE:HD12	2.49	0.48
1:H:452:MET:HE3	1:H:453:THR:H	1.79	0.48
2:I:875:THR:HG23	3:J:57:TRP:CZ2	2.49	0.48
1:C:282:GLN:HE21	1:C:299:TRP:HE1	1.61	0.48
2:D:105:ASP:N	2:D:106:GLY:HA2	2.29	0.48
2:D:652:LEU:HD11	2:D:654:MET:HE2	1.94	0.48
2:D:848:TYR:C	2:D:850:ASP:H	2.17	0.48
2:I:244:ASN:OD1	2:I:245:ILE:N	2.47	0.48
2:I:828:VAL:HG13	2:I:899:LEU:HB3	1.96	0.48
2:B:118:ASP:OD2	2:B:121:ASN:HB2	2.14	0.48
2:B:788:GLU:HA	2:B:894:MET:CE	2.43	0.48
2:B:935:GLY:C	2:B:936:ASN:HD22	2.16	0.48
2:D:489:TYR:CE2	2:D:517:HIS:HB3	2.49	0.48
2:M:776:ARG:HB3	2:M:858:ASN:OD1	2.14	0.48
3:N:57:TRP:HE3	3:N:68:LYS:NZ	2.11	0.48
2:D:531:GLU:HG3	2:D:541:THR:HG22	1.95	0.47
2:I:188:VAL:HG11	2:I:191:LEU:HG	1.96	0.47
2:I:565:THR:HG22	2:I:590:SER:HB2	1.95	0.47
2:M:57:THR:OG1	2:M:59:ASP:O	2.29	0.47
2:M:786:PRO:HB2	2:M:894:MET:SD	2.54	0.47
2:M:867:GLU:N	2:M:867:GLU:OE1	2.47	0.47
2:B:531:GLU:HG3	2:B:541:THR:HG22	1.96	0.47
2:D:105:ASP:OD2	2:D:166:THR:OG1	2.27	0.47
2:M:665:VAL:CG1	2:M:704:LEU:HD13	2.43	0.47
2:M:893:ASP:HB2	2:M:897:CYS:HB2	1.95	0.47
1:A:255:VAL:HG11	1:A:281:GLY:CA	2.43	0.47
2:B:923:LYS:HD2	2:B:923:LYS:N	2.29	0.47
2:D:173:LYS:HA	2:D:174:GLY:HA2	1.64	0.47
2:D:195:GLN:HG2	2:D:197:GLU:H	1.79	0.47
3:J:71:VAL:CG1	3:J:80:PHE:HB2	2.44	0.47
2:M:173:LYS:HA	2:M:174:GLY:HA2	1.60	0.47
1:A:92:LEU:HB3	1:A:101:ARG:HH21	1.79	0.47
2:B:822:ASP:HB2	2:B:908:ARG:HD2	1.94	0.47
1:C:54:GLU:HB2	1:C:301:ASN:OD1	2.14	0.47
1:C:204:THR:O	1:C:208:LYS:HG3	2.15	0.47
2:D:356:PRO:HG2	2:D:424:TYR:CZ	2.49	0.47
1:L:120:SER:HB2	1:L:475:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:419:SER:OG	1:L:422:GLN:HG3	2.15	0.47
3:N:123:GLN:HG2	3:N:132:THR:HG22	1.96	0.47
2:D:473:ASN:HB3	2:D:533:SER:HB3	1.97	0.47
1:H:204:THR:O	1:H:207:VAL:HG12	2.14	0.47
3:J:43:MET:HG3	3:J:59:ASP:O	2.15	0.47
1:L:187:LEU:HD21	1:L:328:LEU:HB3	1.95	0.47
1:L:448:LEU:O	1:L:450:LYS:HG2	2.15	0.47
1:A:153:ASP:OD1	1:A:186:ARG:NH1	2.47	0.47
2:B:207:THR:CB	2:B:210:GLU:HG2	2.43	0.47
3:N:93:SER:OG	3:N:94:LYS:N	2.47	0.47
2:B:380:GLU:OE2	2:I:453:ARG:NH2	2.33	0.47
1:C:198:ILE:HD12	1:C:476:TRP:HZ3	1.80	0.47
1:C:375:SER:C	1:C:377:ALA:H	2.17	0.47
2:D:981:MET:CE	2:D:983:LYS:HB2	2.44	0.47
1:H:171:PHE:CZ	1:H:221:VAL:HG22	2.49	0.47
2:I:441:SER:HA	2:I:442:GLY:HA2	1.60	0.47
2:I:741:ILE:HG13	2:I:756:ILE:HG12	1.97	0.47
2:I:862:LYS:HD3	2:I:871:TYR:CE2	2.49	0.47
3:J:143:PHE:HB3	3:J:144:PRO:HD2	1.97	0.47
1:L:56:ASN:HB3	1:L:59:ASN:HD21	1.80	0.47
1:L:57:GLN:HE22	4:O:6:GLY:HA2	1.78	0.47
1:A:392:TRP:CD1	1:A:407:ILE:HD11	2.50	0.47
2:D:288:ASP:OD1	2:D:288:ASP:N	2.45	0.47
2:I:56:ARG:NH2	2:I:136:ASP:OD1	2.48	0.47
2:I:282:MET:HE2	2:I:282:MET:HB2	1.56	0.47
1:L:404:TRP:O	1:L:408:ARG:HG3	2.15	0.47
1:A:50:GLU:HG3	1:A:282:GLN:NE2	2.30	0.47
2:B:884:TYR:CG	2:B:885:LYS:N	2.83	0.47
2:B:938:LEU:HA	2:B:938:LEU:HD23	1.67	0.47
2:I:104:VAL:O	2:I:164:ILE:O	2.33	0.47
1:L:374:TRP:HZ3	1:L:387:ILE:HD11	1.80	0.47
2:M:863:ILE:HB	2:M:870:THR:CG2	2.44	0.47
2:B:320:ASN:OD1	2:B:378:GLU:HG3	2.15	0.47
1:C:373:ALA:O	1:C:375:SER:N	2.48	0.47
2:D:561:TYR:CD2	2:D:594:THR:HA	2.49	0.47
2:D:702:ILE:O	2:D:702:ILE:HG13	2.15	0.47
2:D:850:ASP:OD2	3:E:14:LYS:HE2	2.15	0.47
2:M:798:MET:O	2:M:902:LYS:NZ	2.26	0.47
3:N:71:VAL:HG11	3:N:80:PHE:CD1	2.50	0.47
2:B:469:VAL:O	2:B:472:PHE:HB2	2.15	0.46
1:H:34:VAL:CG1	1:H:114:ILE:HD13	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:ASN:HB3	1:L:59:ASN:ND2	2.30	0.46
1:L:142:GLU:O	1:L:146:LYS:HB3	2.15	0.46
2:M:158:ALA:HB2	2:M:594:THR:HG21	1.97	0.46
1:L:156:GLU:O	1:L:159:LEU:HD13	2.15	0.46
3:N:85:PHE:CG	3:N:96:LYS:HG2	2.50	0.46
2:B:530:PHE:HB3	2:B:542:VAL:HG22	1.97	0.46
2:B:583:THR:HG1	2:B:658:LYS:H	1.59	0.46
2:B:773:PRO:HD2	2:B:871:TYR:CE1	2.51	0.46
1:C:315:LYS:HG3	1:C:316:PRO:HD2	1.97	0.46
1:C:409:ARG:HE	1:C:410:THR:HG23	1.80	0.46
1:C:444:GLU:HB3	2:D:864:VAL:HG11	1.97	0.46
1:H:431:THR:O	1:H:434:GLU:HG2	2.15	0.46
1:L:77:TYR:CE2	2:M:683:PRO:HG2	2.50	0.46
1:L:187:LEU:HD12	1:L:216:PHE:CZ	2.50	0.46
1:L:238:ASN:O	1:L:242:VAL:HG22	2.15	0.46
2:B:311:SER:O	2:B:386:GLY:HA2	2.16	0.46
1:H:456:LEU:O	1:H:460:GLN:HG2	2.15	0.46
2:M:824:ARG:HG3	2:M:904:TYR:CZ	2.50	0.46
3:N:120:TYR:CE2	3:N:135:VAL:HG21	2.50	0.46
1:L:255:VAL:HG11	1:L:281:GLY:CA	2.45	0.46
2:M:169:GLY:HA3	2:M:269:ASP:HB2	1.96	0.46
2:M:257:ASN:HB2	2:M:276:GLN:OE1	2.16	0.46
1:A:97:ASN:ND2	1:A:165[B]:ASP:OD1	2.39	0.46
2:B:829:MET:HB2	2:B:829:MET:HE3	1.79	0.46
2:D:505:LEU:HD12	2:M:516:GLN:HB3	1.97	0.46
3:F:116:ASP:OD2	3:F:139:ARG:NH2	2.31	0.46
2:I:298:ARG:HG2	2:I:311:SER:OG	2.16	0.46
2:I:890:GLY:HA3	2:I:894:MET:O	2.15	0.46
3:J:96:LYS:HE2	3:J:96:LYS:HB3	1.64	0.46
2:M:356:PRO:HG2	2:M:424:TYR:CZ	2.50	0.46
2:M:554:LYS:HG3	2:M:557:ARG:NH2	2.30	0.46
2:M:855:ILE:HG23	2:M:874:ASN:ND2	2.30	0.46
3:N:94:LYS:HB2	3:N:125:ASP:HB2	1.97	0.46
1:A:37:GLU:HG2	1:A:76:SER:OG	2.16	0.46
2:B:212:GLY:HA2	2:B:840:THR:HG23	1.96	0.46
2:B:938:LEU:O	2:B:974:ARG:NH1	2.48	0.46
1:C:69:SER:O	2:D:749:GLY:HA2	2.16	0.46
1:C:144:VAL:O	1:C:148:ILE:HG12	2.16	0.46
2:D:99:GLN:NE2	2:D:959:ASP:OD2	2.48	0.46
2:I:581:VAL:HG13	2:I:657:PHE:CE1	2.51	0.46
2:I:837:ASN:HA	2:I:840:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:263:ASP:O	1:L:266:ILE:HB	2.15	0.46
1:L:364:GLU:OE1	1:L:364:GLU:N	2.45	0.46
1:L:367:ILE:HG23	1:L:372:CYS:HB2	1.98	0.46
2:M:361:THR:HA	2:M:362:PRO:HD3	1.76	0.46
2:M:441:SER:HA	2:M:442:GLY:HA2	1.61	0.46
2:B:312:LEU:HD22	2:B:384:PHE:CZ	2.50	0.46
1:C:352:THR:HG22	1:C:364:GLU:HG3	1.98	0.46
2:I:84:ASN:HD22	2:I:131:ASN:HD21	1.62	0.46
2:I:743:THR:HG21	4:K:1:GLY:HA3	1.97	0.46
1:L:312:GLY:HA2	1:L:315:LYS:HB3	1.98	0.46
3:N:62:GLY:HA2	3:N:66:GLU:HA	1.98	0.46
2:B:116:SER:HB2	2:B:124:TYR:CD2	2.51	0.46
2:M:773:PRO:HD3	2:M:871:TYR:CE2	2.51	0.46
2:M:863:ILE:O	2:M:870:THR:HG22	2.16	0.46
2:B:333:SER:OG	2:B:366:MET:O	2.17	0.46
2:D:635:LEU:HD13	2:D:687:TYR:CE2	2.51	0.46
2:D:741:ILE:HD11	2:D:754:TYR:CD1	2.51	0.46
1:H:39:TYR:OH	1:H:397:TYR:HA	2.16	0.46
1:L:258:LEU:CB	1:L:266:ILE:HD13	2.46	0.46
1:L:263:ASP:HA	1:L:367:ILE:HD11	1.97	0.45
1:L:329:ILE:O	1:L:332:VAL:HG12	2.16	0.45
2:M:643:GLU:HG2	2:M:644:MET:N	2.31	0.45
1:A:276:ASP:HB3	1:A:278:LYS:HE2	1.97	0.45
2:B:504:ASN:OD1	2:B:506:LYS:HG2	2.15	0.45
1:C:53:PRO:HD2	1:C:301:ASN:ND2	2.31	0.45
2:D:475:ASN:HB3	2:D:531:GLU:HB3	1.97	0.45
2:I:762:GLY:HA3	2:I:798:MET:HG2	1.96	0.45
3:J:83:THR:O	3:J:83:THR:OG1	2.33	0.45
1:L:68:GLU:OE1	1:L:459:ARG:HD2	2.17	0.45
1:L:245:THR:HB	2:M:437:SER:HA	1.98	0.45
1:L:414:LYS:O	1:L:434:GLU:HB2	2.16	0.45
1:L:427:GLU:H	1:L:427:GLU:HG3	1.54	0.45
2:M:190:ARG:NH2	2:M:947:THR:HA	2.26	0.45
2:B:938:LEU:O	2:B:939:PHE:CD1	2.69	0.45
2:D:347:GLU:HG3	2:D:369:TYR:CD1	2.51	0.45
2:D:429:PRO:O	2:D:434:GLN:HG2	2.17	0.45
3:J:94:LYS:HB2	3:J:125:ASP:HB2	1.98	0.45
1:L:476:TRP:CZ2	1:L:477:TRP:HD1	2.34	0.45
2:M:195:GLN:O	2:M:339:ARG:HD3	2.16	0.45
2:M:772:ASP:HB2	2:M:871:TYR:CE2	2.51	0.45
3:N:68:LYS:HZ2	3:N:69:LEU:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:GLU:HB3	2:B:911:VAL:HG11	1.98	0.45
1:H:208:LYS:HD2	1:H:336:PHE:HB3	1.98	0.45
2:I:180:ASN:HB2	2:I:258:SER:HB3	1.98	0.45
1:L:280:VAL:O	1:L:305:SER:HB2	2.17	0.45
1:L:344:LYS:HG3	1:L:374:TRP:CD1	2.52	0.45
2:B:338:PRO:HB2	2:B:341:ILE:HD12	1.98	0.45
1:C:18:THR:OG1	1:C:19:ALA:N	2.49	0.45
1:C:469:VAL:HB	1:C:473:THR:HG21	1.97	0.45
2:D:41:GLY:HA3	2:D:565:THR:HB	1.99	0.45
2:D:834:LYS:HE2	2:D:897:CYS:SG	2.56	0.45
3:E:57:TRP:CZ2	3:E:70:LYS:HE3	2.51	0.45
2:I:58:SER:HB2	2:I:277:ILE:HD12	1.99	0.45
2:B:497:LEU:HA	2:B:507:ASN:O	2.17	0.45
1:C:331:GLU:O	1:C:335:ARG:HB3	2.16	0.45
2:D:785:LEU:HD23	2:D:878:ILE:HD13	1.99	0.45
3:E:12:VAL:HA	3:E:75:TYR:CE1	2.52	0.45
1:H:102:PHE:CZ	1:H:106:ILE:HD11	2.51	0.45
1:H:372:CYS:HB3	1:H:386:LEU:HD11	1.97	0.45
3:J:27:ILE:HD12	3:J:28:ASP:H	1.81	0.45
1:L:379:THR:HB	1:L:382:ASP:H	1.82	0.45
2:M:56:ARG:HD2	2:M:979:ASN:ND2	2.32	0.45
2:M:574:LEU:HB3	2:M:579:GLN:HB3	1.98	0.45
2:M:777:ILE:HD11	2:M:786:PRO:HB3	1.97	0.45
2:B:451:ILE:HG21	2:I:451:ILE:HG21	1.98	0.45
2:M:938:LEU:O	2:M:939:PHE:CD1	2.69	0.45
2:B:582:ILE:HD13	2:B:656:PHE:HD1	1.82	0.45
2:D:497:LEU:HA	2:D:507:ASN:O	2.17	0.45
2:I:195:GLN:O	2:I:339:ARG:HG3	2.16	0.45
2:I:213:SER:OG	2:I:842:ASN:ND2	2.49	0.45
3:N:58:LEU:H	3:N:68:LYS:HZ1	1.65	0.45
1:A:273:THR:HG23	1:A:278:LYS:O	2.17	0.45
2:B:545:ARG:HG2	2:B:561:TYR:CZ	2.52	0.45
1:C:73:MET:O	1:C:73:MET:HG2	2.16	0.45
2:I:697:ILE:HD13	2:I:731:VAL:HG13	1.99	0.45
1:A:35:GLY:O	1:A:236:TRP:HB2	2.18	0.45
2:B:198:PHE:CE1	2:B:851:ARG:HD2	2.52	0.45
2:B:305:ALA:HB1	2:B:393:GLU:O	2.16	0.45
2:D:105:ASP:H	2:D:107:VAL:H	1.64	0.45
2:I:64:LEU:HD22	2:I:68:ILE:HD11	1.99	0.45
3:J:71:VAL:HG11	3:J:80:PHE:HB2	1.99	0.45
1:A:105:THR:HA	1:A:108:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:CD2	1:A:186:ARG:HG2	2.47	0.44
2:B:569:ILE:HD13	2:B:584:PHE:CE1	2.52	0.44
2:B:663:PHE:HB2	2:B:706:ILE:HG22	1.99	0.44
1:C:24:PRO:HG3	1:C:167:PRO:HB2	1.99	0.44
2:D:312:LEU:HD11	2:M:295:PHE:HE1	1.82	0.44
2:D:333:SER:HG	2:D:366:MET:N	2.14	0.44
2:D:767:GLN:CG	2:D:895:GLY:H	2.23	0.44
2:I:332:ASN:OD1	2:I:832:ARG:NH2	2.50	0.44
3:J:16:ALA:O	3:J:139:ARG:NH1	2.49	0.44
1:L:32:SER:HA	1:L:235:PRO:HG3	1.99	0.44
1:L:476:TRP:CH2	1:L:477:TRP:HB3	2.53	0.44
2:B:253:PHE:CD1	2:B:254:ARG:N	2.85	0.44
2:B:845:GLN:HE22	2:B:947:THR:CG2	2.26	0.44
1:C:229:GLU:O	1:C:233:ARG:CZ	2.65	0.44
2:D:785:LEU:HD23	2:D:878:ILE:HD12	1.98	0.44
2:I:195:GLN:HB2	2:I:844:ILE:HA	1.98	0.44
2:I:331:LEU:HD12	2:I:331:LEU:HA	1.78	0.44
1:L:188:ARG:NE	1:L:402:GLU:OE2	2.49	0.44
1:L:209:THR:O	1:L:210:LEU:HD12	2.17	0.44
2:M:338:PRO:HG2	2:M:341:ILE:HG13	1.98	0.44
2:M:740:GLY:O	2:M:757:THR:HG23	2.17	0.44
3:N:101:LYS:HD2	3:N:103:LEU:HD11	1.98	0.44
1:A:462:ASN:HB3	1:A:465:THR:HG23	1.99	0.44
2:B:312:LEU:HB2	2:I:312:LEU:HD12	1.98	0.44
1:C:160:ASP:OD1	1:C:160:ASP:N	2.49	0.44
2:D:955:SER:HB2	2:D:956:PHE:CE1	2.52	0.44
2:I:539:TYR:HB2	2:I:567:SER:HB3	1.99	0.44
2:M:111:ASN:OD1	2:M:128:ASN:ND2	2.50	0.44
3:N:58:LEU:HD21	3:N:120:TYR:OH	2.17	0.44
1:A:12:PRO:HB3	2:I:499:ILE:HD13	1.99	0.44
1:A:87:ASP:O	1:A:91:VAL:HG23	2.17	0.44
1:A:123:PRO:HD3	1:A:138:TRP:CE2	2.53	0.44
2:B:559:PHE:HB3	2:B:642:PRO:HG3	2.00	0.44
2:D:394:PHE:HD2	2:D:395:LEU:HG	1.82	0.44
1:L:349:ALA:HA	1:L:352:THR:OG1	2.17	0.44
1:L:456:LEU:HD12	1:L:459:ARG:HB3	1.99	0.44
2:M:406:LEU:HD13	2:M:457:ILE:CD1	2.48	0.44
2:M:575:ASN:HB2	2:M:578:LEU:HB3	1.98	0.44
2:B:68:ILE:HB	2:B:71:VAL:HG22	1.99	0.44
2:B:105:ASP:N	2:B:106:GLY:HA2	2.33	0.44
2:B:530:PHE:O	2:B:541:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:675:GLN:NE2	2:B:697:ILE:HD13	2.33	0.44
1:C:430:TYR:CE2	1:C:432:PRO:HA	2.53	0.44
2:D:441:SER:HA	2:D:442:GLY:HA2	1.68	0.44
2:I:561:TYR:CD2	2:I:594:THR:HA	2.52	0.44
2:I:884:TYR:CG	2:I:885:LYS:N	2.86	0.44
1:L:268:TYR:CZ	1:L:311:ILE:HD12	2.52	0.44
2:M:534:TRP:HD1	2:M:535:LYS:N	2.15	0.44
2:B:398:PHE:HA	2:B:464:ASN:O	2.18	0.44
2:B:537:MET:HA	2:B:569:ILE:HG23	2.00	0.44
1:C:348:GLU:O	1:C:352:THR:HG23	2.18	0.44
2:D:120:LEU:HA	2:D:967:TYR:CD2	2.52	0.44
2:D:134:ASN:ND2	2:D:275:SER:HB3	2.32	0.44
2:D:588:ARG:NH2	2:D:664:ASP:OD1	2.49	0.44
1:L:229:GLU:O	1:L:233:ARG:NH2	2.51	0.44
1:L:470:PRO:HD2	1:L:473:THR:HG21	2.00	0.44
2:M:101:LEU:HD11	2:M:108:PRO:HB3	1.98	0.44
2:M:752:SER:HB2	2:M:754:TYR:CE1	2.53	0.44
2:M:788:GLU:HG2	2:M:789:ALA:O	2.18	0.44
1:C:219:GLY:O	1:C:322:GLN:HB2	2.18	0.44
2:D:654:MET:HB2	2:D:663:PHE:CE2	2.53	0.44
2:D:660:ARG:HE	2:D:660:ARG:HB3	1.68	0.44
2:D:848:TYR:O	2:D:850:ASP:N	2.49	0.44
2:I:770:GLU:OE2	2:I:862:LYS:HE2	2.18	0.44
1:A:23:PHE:HE2	1:A:104:THR:HG22	1.81	0.44
1:C:412:CYS:HA	1:C:413:PRO:C	2.39	0.44
2:D:94:LEU:HD23	2:D:94:LEU:HA	1.58	0.44
2:D:568:PHE:CE2	2:D:570:PHE:HB3	2.53	0.44
2:D:877:PRO:HG3	3:E:46:TYR:CZ	2.53	0.44
2:I:412:GLN:HB2	2:I:451:ILE:HD13	2.00	0.44
1:L:224:ASP:CG	1:L:316:PRO:HG3	2.38	0.44
1:L:386:LEU:HD12	1:L:386:LEU:HA	1.67	0.44
1:A:54:GLU:OE2	1:A:300:LYS:HB3	2.17	0.43
2:B:394:PHE:CD2	2:B:395:LEU:HG	2.52	0.43
2:B:429:PRO:O	2:B:434:GLN:HG2	2.17	0.43
1:C:470:PRO:O	1:C:473:THR:HG23	2.18	0.43
2:M:155:SER:OG	2:M:156:ARG:N	2.51	0.43
2:M:170:ARG:HD3	2:M:262:ASN:HD21	1.83	0.43
2:M:267:LYS:HA	2:M:267:LYS:HD3	1.76	0.43
1:A:102:PHE:CZ	1:A:106:ILE:HD11	2.53	0.43
1:A:192:ARG:HD3	1:A:409:ARG:HD3	1.99	0.43
1:A:449:MET:CE	1:A:471:GLY:HA3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLU:HA	2:B:541:THR:HG22	1.99	0.43
2:B:835:ASP:HA	2:B:898:PHE:CE1	2.54	0.43
1:H:461:GLN:NE2	2:I:741:ILE:O	2.51	0.43
1:L:142:GLU:OE2	1:L:142:GLU:N	2.52	0.43
1:L:191:LEU:HD23	1:L:191:LEU:HA	1.81	0.43
1:L:321:THR:HB	1:L:324:GLU:HB2	2.00	0.43
1:L:470:PRO:HD2	1:L:473:THR:CG2	2.47	0.43
2:M:56:ARG:HH22	2:M:136:ASP:CG	2.21	0.43
2:M:332:ASN:OD1	2:M:832:ARG:NH2	2.51	0.43
2:M:824:ARG:NH1	2:M:904:TYR:OH	2.51	0.43
2:B:155:SER:HB2	2:B:596:ASN:HA	2.00	0.43
1:C:32:SER:HB2	1:C:79:ILE:HD12	2.00	0.43
2:D:751:THR:HG21	2:D:899:LEU:HD21	2.00	0.43
3:F:20:TRP:CD1	3:F:140:ARG:HG3	2.53	0.43
3:F:48:THR:HG21	3:F:55:GLU:HG3	2.00	0.43
1:H:449:MET:HE3	1:H:451:ARG:H	1.83	0.43
2:I:753:MET:HE3	2:I:753:MET:HB2	1.77	0.43
1:L:52:LYS:HB3	1:L:301:ASN:HD21	1.83	0.43
1:L:73:MET:HE2	1:L:455:PRO:HD3	1.99	0.43
2:M:923:LYS:HZ3	2:M:924:THR:CG2	2.27	0.43
2:B:531:GLU:HG3	2:B:541:THR:CG2	2.47	0.43
1:C:20:ASP:HB2	1:C:167:PRO:HD3	2.00	0.43
2:D:291:ASP:O	2:D:317:GLN:HA	2.18	0.43
2:I:126:PHE:CE1	2:I:321:PHE:HB2	2.53	0.43
2:I:230:ASN:O	2:I:231:ASN:HB3	2.18	0.43
1:L:333:TYR:HD1	1:L:337:HIS:ND1	2.16	0.43
2:M:730:LYS:HG2	2:M:732:ILE:HD13	1.99	0.43
2:M:753:MET:HE3	2:M:764:PHE:CZ	2.53	0.43
2:M:776:ARG:HG3	2:M:860:VAL:CG1	2.48	0.43
1:C:54:GLU:OE2	1:C:300:LYS:HB3	2.18	0.43
2:D:412:GLN:HA	2:D:450:GLN:O	2.19	0.43
3:F:93:SER:OG	3:F:94:LYS:N	2.48	0.43
1:H:153:ASP:OD1	1:H:186:ARG:NH2	2.41	0.43
2:I:282:MET:H	2:I:282:MET:HG3	1.56	0.43
2:I:577:ASN:HB3	2:I:578:LEU:H	1.55	0.43
2:I:834:LYS:HG3	2:I:948:PHE:CZ	2.54	0.43
2:M:658:LYS:O	2:M:658:LYS:HD3	2.18	0.43
3:N:43:MET:HB2	3:N:59:ASP:O	2.18	0.43
1:A:49:TYR:CE2	1:A:400:HIS:HE1	2.36	0.43
2:B:384:PHE:HE2	2:B:406:LEU:HD23	1.83	0.43
3:E:21:VAL:HG21	3:E:43:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:485:ARG:NH1	2:I:521:ARG:HD3	2.33	0.43
1:L:383:LYS:O	1:L:387:ILE:HG12	2.18	0.43
2:M:667:TYR:OH	2:M:700:ARG:HD2	2.18	0.43
2:M:718:TRP:CD1	2:M:810:LEU:HD21	2.53	0.43
3:N:71:VAL:HG12	3:N:80:PHE:HB2	2.00	0.43
3:F:91:TYR:O	3:F:91:TYR:CD2	2.72	0.43
2:I:302:LYS:HA	2:I:307:THR:HA	2.01	0.43
1:L:159:LEU:CD2	1:L:175:ILE:HD11	2.49	0.43
1:A:164:MET:HE3	1:A:173:LYS:HA	2.00	0.43
1:A:237:TYR:CD2	1:A:313:ALA:HA	2.53	0.43
2:B:94:LEU:O	2:B:960:LEU:HD23	2.18	0.43
2:B:767:GLN:HG3	2:B:788:GLU:HG3	2.01	0.43
2:B:767:GLN:HE21	2:B:788:GLU:CD	2.21	0.43
2:D:730:LYS:HG3	2:D:731:VAL:O	2.19	0.43
1:H:347:TYR:HD1	1:H:387:ILE:HG22	1.83	0.43
1:L:159:LEU:HD23	1:L:175:ILE:HD11	2.00	0.43
1:L:344:LYS:HG3	1:L:374:TRP:CG	2.53	0.43
2:M:499:ILE:O	2:M:507:ASN:ND2	2.43	0.43
1:C:102:PHE:CZ	1:C:106:ILE:HD11	2.53	0.43
1:C:116:VAL:HG21	1:C:144:VAL:CG2	2.48	0.43
1:C:252:TYR:HB3	1:C:253:PRO:HD3	2.01	0.43
1:C:260:SER:OG	1:C:432:PRO:HG2	2.18	0.43
2:D:410:THR:OG1	2:M:410:THR:HG21	2.19	0.43
2:I:666:SER:O	2:I:702:ILE:HA	2.19	0.43
1:L:416:SER:O	1:L:418:TYR:N	2.52	0.43
2:M:610:SER:CB	2:M:630:SER:HB2	2.49	0.43
2:B:68:ILE:HB	2:B:71:VAL:HG21	2.01	0.43
2:B:726:LYS:HZ2	2:B:726:LYS:HG2	1.55	0.43
1:C:237:TYR:CD2	1:C:313:ALA:HA	2.54	0.43
2:D:244:ASN:OD1	2:D:245:ILE:N	2.51	0.43
3:F:21:VAL:HG11	3:F:43:MET:HE1	2.00	0.43
1:H:391:LYS:O	1:H:395:LEU:HG	2.19	0.43
2:I:402:TYR:HD1	2:I:461:ILE:HG12	1.83	0.43
2:B:50:GLU:HG2	2:B:54:GLU:OE2	2.19	0.42
2:B:109:LEU:HD22	2:B:133:ILE:HD11	2.01	0.42
2:B:298:ARG:HG2	2:B:311:SER:OG	2.18	0.42
2:D:296:SER:OG	2:D:298:ARG:NH1	2.52	0.42
3:F:85:PHE:HB3	3:F:94:LYS:CD	2.49	0.42
1:H:188:ARG:CZ	1:H:402:GLU:OE2	2.67	0.42
1:L:88:ALA:O	1:L:92:LEU:HD23	2.19	0.42
2:M:312:LEU:HD22	2:M:384:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:475:ASN:HB3	2:M:531:GLU:HG2	1.99	0.42
3:F:101:LYS:HG3	3:F:119:VAL:HG23	2.01	0.42
1:H:169:LEU:H	1:H:169:LEU:HD12	1.84	0.42
1:H:183:ASN:OD1	1:H:186:ARG:NH1	2.52	0.42
2:I:667:TYR:OH	2:I:700:ARG:HD2	2.19	0.42
2:M:326:GLN:HE22	4:O:5:GLY:HA2	1.83	0.42
1:A:89:LYS:O	1:A:93:GLU:HG3	2.18	0.42
2:D:39:ALA:HB1	2:D:539:TYR:CG	2.54	0.42
2:D:444:THR:O	2:D:496:ASP:HA	2.19	0.42
1:H:386:LEU:HD12	1:H:386:LEU:HA	1.72	0.42
1:H:454:TYR:CE1	1:H:466:PRO:HG2	2.54	0.42
2:I:105:ASP:H	2:I:107:VAL:H	1.66	0.42
1:L:389:MET:O	1:L:393:VAL:HG23	2.19	0.42
2:M:202:TRP:HA	2:M:214:TRP:HB2	2.01	0.42
2:M:421:TYR:HD1	2:M:421:TYR:C	2.23	0.42
2:M:545:ARG:HG2	2:M:561:TYR:CZ	2.53	0.42
2:M:863:ILE:HB	2:M:870:THR:HG22	2.01	0.42
1:A:23:PHE:CD2	1:A:104:THR:HG22	2.54	0.42
1:A:412:CYS:HA	1:A:413:PRO:C	2.40	0.42
2:I:275:SER:OG	2:I:294:THR:HG22	2.20	0.42
2:I:700:ARG:HH11	2:I:700:ARG:HD3	1.70	0.42
1:L:257:TYR:CE1	1:L:389:MET:HE2	2.55	0.42
3:N:69:LEU:HD21	3:N:97:ILE:HD11	2.02	0.42
1:A:230:THR:O	1:A:232:LYS:HG2	2.19	0.42
2:B:658:LYS:O	2:B:659:ASN:HB2	2.19	0.42
2:B:834:LYS:HD3	2:B:898:PHE:CD1	2.55	0.42
2:D:385:TYR:HA	2:D:406:LEU:O	2.19	0.42
2:I:819:ILE:HG23	2:I:910:VAL:HG22	2.02	0.42
1:L:289:HIS:O	1:L:293:ILE:HG13	2.19	0.42
1:L:415:LEU:HD11	1:L:437:ALA:HB2	2.01	0.42
2:M:39:ALA:HB1	2:M:539:TYR:CG	2.54	0.42
2:M:534:TRP:CD1	2:M:534:TRP:C	2.93	0.42
2:M:834:LYS:HE3	2:M:948:PHE:CE2	2.55	0.42
2:B:195:GLN:HG2	2:B:196:ASN:N	2.33	0.42
1:C:57:GLN:OE1	4:G:6:GLY:HA2	2.19	0.42
1:C:75:TYR:O	1:C:79:ILE:HG23	2.18	0.42
2:D:516:GLN:HB3	2:M:505:LEU:HD12	2.01	0.42
1:H:375:SER:C	1:H:377:ALA:H	2.23	0.42
2:M:657:PHE:O	2:M:658:LYS:HB3	2.20	0.42
2:B:295:PHE:CE2	2:I:312:LEU:HD21	2.54	0.42
2:B:479:GLY:HA3	2:B:527:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:TRP:CZ3	1:H:12:PRO:HG3	2.54	0.42
1:C:451:ARG:NH2	1:C:454:TYR:OH	2.53	0.42
2:D:67:LYS:HE3	2:D:820:ASP:CG	2.40	0.42
2:D:527:PHE:HB3	2:D:545:ARG:HD3	2.01	0.42
3:F:23:VAL:HG11	3:F:64:PHE:CZ	2.54	0.42
1:H:321:THR:CG2	1:H:324:GLU:H	2.32	0.42
2:M:51:LYS:O	2:M:54:GLU:HG2	2.20	0.42
2:M:534:TRP:HD1	2:M:535:LYS:CB	2.33	0.42
2:M:917:PRO:HG2	2:M:920:TRP:CD2	2.54	0.42
3:N:65:TRP:NE1	3:N:91:TYR:OH	2.40	0.42
2:B:221:SER:O	2:B:237:PRO:HA	2.19	0.42
1:C:43:GLY:HA3	1:C:49:TYR:CZ	2.55	0.42
2:D:53:ALA:O	2:D:56:ARG:HD2	2.20	0.42
2:I:254:ARG:HA	2:I:278:SER:O	2.20	0.42
2:I:362:PRO:O	2:I:439:PRO:HD3	2.20	0.42
2:M:92:SER:HB3	2:M:672:THR:OG1	2.20	0.42
2:M:419:ASN:HB3	2:M:500:PRO:HB3	2.02	0.42
2:M:489:TYR:CE2	2:M:517:HIS:HB3	2.54	0.42
2:M:938:LEU:HD23	2:M:938:LEU:HA	1.87	0.42
1:A:10:ASN:OD1	2:B:517:HIS:HA	2.20	0.42
1:A:101:ARG:O	1:A:105:THR:HG23	2.19	0.42
2:B:95:SER:HB2	2:B:677:PHE:HE2	1.85	0.42
2:B:306:LEU:HD11	2:B:390:LEU:HD11	2.01	0.42
2:B:623:LEU:HA	2:B:624:GLY:HA2	1.83	0.42
2:D:753:MET:CE	2:D:764:PHE:CZ	3.03	0.42
3:E:21:VAL:HG11	3:E:43:MET:HE1	2.02	0.42
1:H:192:ARG:HG2	1:H:409:ARG:HD2	2.01	0.42
1:H:229:GLU:O	1:H:233:ARG:NH2	2.52	0.42
2:I:92:SER:HB3	2:I:672:THR:OG1	2.20	0.42
1:L:89:LYS:HE2	1:L:93:GLU:OE2	2.20	0.42
1:L:449:MET:HE1	1:L:451:ARG:O	2.19	0.42
3:N:95:VAL:HG22	3:N:124:PHE:HD2	1.83	0.42
1:H:2:ASP:HB3	2:I:522:ARG:HH21	1.84	0.42
2:I:610:SER:HB2	2:I:621:PHE:CD2	2.55	0.42
1:L:202:SER:O	1:L:205:GLU:HB2	2.20	0.42
2:M:196:ASN:OD1	2:M:339:ARG:NH1	2.53	0.42
3:N:96:LYS:HD3	3:N:96:LYS:HA	1.11	0.42
1:A:20:ASP:OD1	1:A:20:ASP:N	2.53	0.41
2:B:104:VAL:HG22	2:B:164:ILE:HG21	2.00	0.41
1:C:187:LEU:HD12	1:C:207:VAL:HG23	2.01	0.41
1:C:296:THR:CG2	2:D:203:ASN:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:237:TYR:CD2	1:H:313:ALA:HA	2.54	0.41
1:L:87:ASP:OD2	2:M:630:SER:OG	2.31	0.41
1:L:145:TYR:CE2	1:L:189:MET:HG2	2.55	0.41
1:L:171:PHE:CG	1:L:177:GLN:HB3	2.55	0.41
1:L:200:ALA:O	1:L:204:THR:HG22	2.20	0.41
2:M:254:ARG:HA	2:M:278:SER:O	2.19	0.41
2:B:104:VAL:HG22	2:B:164:ILE:CG2	2.50	0.41
2:B:880:SER:HA	2:B:883:ILE:HG12	2.01	0.41
2:B:935:GLY:HA2	2:B:976:PHE:HA	2.02	0.41
2:D:806:VAL:HG22	2:D:821:PHE:HB2	2.01	0.41
1:H:62:CYS:HB3	1:H:287:LYS:HE3	2.01	0.41
1:H:146:LYS:HB2	1:H:146:LYS:HE2	1.68	0.41
1:H:222:LYS:HD3	1:H:224:ASP:HB2	2.01	0.41
2:I:581:VAL:HG13	2:I:657:PHE:HE1	1.83	0.41
1:L:348:GLU:HG2	1:L:368:LEU:HD22	2.02	0.41
2:M:731:VAL:O	2:M:757:THR:O	2.39	0.41
3:N:58:LEU:H	3:N:68:LYS:HZ3	1.67	0.41
2:D:314:TYR:CZ	2:M:406:LEU:HD21	2.55	0.41
2:D:332:ASN:OD1	2:D:832:ARG:NH2	2.53	0.41
2:D:384:PHE:HE2	2:D:406:LEU:HD23	1.84	0.41
2:M:421:TYR:C	2:M:421:TYR:CD1	2.93	0.41
2:M:429:PRO:O	2:M:434:GLN:HG2	2.20	0.41
2:M:575:ASN:HB2	2:M:578:LEU:CB	2.50	0.41
1:C:263:ASP:OD1	1:C:265:ARG:HD2	2.20	0.41
2:I:58:SER:HB3	2:I:254:ARG:NH1	2.35	0.41
2:I:611:SER:HB2	2:I:620:THR:HG22	2.02	0.41
2:I:683:PRO:HG3	2:I:688:THR:HG22	2.02	0.41
1:L:335:ARG:HG3	1:L:384:LEU:HD21	2.02	0.41
1:A:69:SER:O	2:B:749:GLY:HA2	2.21	0.41
1:A:116:VAL:HG21	1:A:144:VAL:CG2	2.50	0.41
2:B:806:VAL:HG22	2:B:821:PHE:HB2	2.01	0.41
2:D:332:ASN:O	2:D:336:GLN:HG3	2.20	0.41
2:D:623:LEU:HA	2:D:624:GLY:HA2	1.87	0.41
1:H:331:GLU:HG3	1:H:335:ARG:HD3	2.03	0.41
2:I:219:ASP:OD1	2:I:220:GLY:N	2.53	0.41
2:I:862:LYS:HD3	2:I:871:TYR:CZ	2.55	0.41
2:B:71:VAL:HG11	2:B:143:ILE:HG21	2.03	0.41
2:B:91:VAL:HG13	2:B:98:ASN:ND2	2.35	0.41
2:B:713:THR:HG22	2:B:714:LYS:N	2.34	0.41
2:D:194:PHE:CZ	2:D:245:ILE:HD12	2.55	0.41
2:D:464:ASN:HD22	2:D:477:LEU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:GLN:OE1	1:H:218:THR:HB	2.20	0.41
2:I:175:VAL:HG23	2:I:177:ILE:HG13	2.02	0.41
1:L:257:TYR:HB2	1:L:433:GLY:CA	2.50	0.41
1:L:412:CYS:HA	1:L:413:PRO:C	2.41	0.41
2:M:554:LYS:HB2	2:M:554:LYS:HE3	1.63	0.41
2:M:776:ARG:HG3	2:M:860:VAL:HG11	2.03	0.41
1:A:69:SER:HA	1:A:456:LEU:HD22	2.03	0.41
2:B:183:VAL:HG13	2:B:253:PHE:CE1	2.56	0.41
2:B:244:ASN:OD1	2:B:245:ILE:N	2.54	0.41
2:B:489:TYR:CE2	2:B:517:HIS:HB3	2.56	0.41
2:D:152:LEU:HD12	2:D:152:LEU:HA	1.83	0.41
2:D:289:SER:HB2	2:D:320:ASN:HB2	2.02	0.41
2:D:770:GLU:HG2	2:D:771:ARG:N	2.36	0.41
3:E:15:MET:SD	3:E:78:ARG:HA	2.60	0.41
1:H:106:ILE:CD1	1:H:182:ALA:HB2	2.51	0.41
2:I:849:ASN:ND2	2:I:849:ASN:O	2.53	0.41
2:M:518:MET:HG2	2:M:519:GLU:N	2.35	0.41
3:N:86:VAL:HG12	3:N:87:ASP:N	2.36	0.41
2:B:54:GLU:O	2:B:56:ARG:HG2	2.20	0.41
2:B:900:VAL:HG13	2:B:946:ASN:HB2	2.03	0.41
1:C:97:ASN:O	1:C:101:ARG:HG2	2.21	0.41
2:I:323:THR:O	2:I:329:SER:HB2	2.21	0.41
3:J:43:MET:HE2	3:J:43:MET:HB3	1.95	0.41
1:A:91:VAL:HG11	1:A:104:THR:HG21	2.03	0.41
1:A:190:TYR:CB	1:A:207:VAL:HG23	2.51	0.41
2:B:153:TYR:HB2	2:B:157:ALA:HB2	2.02	0.41
2:B:218:PHE:CE2	2:B:240:ALA:HB2	2.55	0.41
2:B:569:ILE:HD11	2:B:571:SER:OG	2.20	0.41
2:B:677:PHE:HB3	2:B:694:LEU:HD21	2.02	0.41
2:D:527:PHE:HB3	2:D:545:ARG:CD	2.51	0.41
2:D:718:TRP:CD1	2:D:718:TRP:C	2.94	0.41
1:H:164:MET:CE	1:H:173:LYS:HA	2.51	0.41
1:H:252:TYR:N	1:H:253:PRO:HD2	2.35	0.41
1:H:287:LYS:O	1:H:291:GLN:HG2	2.21	0.41
1:H:392:TRP:CD1	1:H:407:ILE:HD11	2.56	0.41
1:H:430:TYR:CE2	1:H:432:PRO:HA	2.55	0.41
2:I:357:GLY:O	2:I:429:PRO:HD2	2.21	0.41
3:J:87:ASP:OD1	3:J:94:LYS:HE3	2.20	0.41
1:L:414:LYS:HD2	1:L:414:LYS:HA	1.84	0.41
1:L:454:TYR:N	1:L:454:TYR:CD1	2.88	0.41
2:M:834:LYS:HG3	2:M:948:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:78:ARG:HB3	3:N:102:VAL:O	2.21	0.41
1:A:265:ARG:HD2	1:A:355:PHE:CZ	2.56	0.41
1:H:110:TYR:CZ	1:H:114:ILE:HD11	2.56	0.41
1:H:327:PHE:CD2	1:H:391:LYS:HA	2.56	0.41
1:H:452:MET:HE3	1:H:453:THR:HG23	2.03	0.41
2:I:56:ARG:O	2:I:254:ARG:NH2	2.48	0.41
2:I:173:LYS:HA	2:I:174:GLY:HA2	1.70	0.41
3:J:6:GLU:OE2	3:J:7:PRO:HD2	2.21	0.41
1:L:142:GLU:N	1:L:142:GLU:CD	2.74	0.41
1:L:347:TYR:CD1	1:L:387:ILE:HD13	2.56	0.41
1:L:347:TYR:HD1	1:L:387:ILE:HD13	1.86	0.41
2:M:144:LEU:HB2	2:M:161:VAL:HB	2.03	0.41
2:M:150:THR:HB	2:M:157:ALA:HB3	2.03	0.41
3:N:58:LEU:HD21	3:N:120:TYR:CZ	2.56	0.41
1:A:126:GLU:O	1:A:136:PRO:HB3	2.21	0.40
2:B:329:SER:O	2:B:333:SER:HB2	2.21	0.40
2:D:976:PHE:CD1	2:D:976:PHE:N	2.89	0.40
3:E:85:PHE:HB3	3:E:94:LYS:HG3	2.03	0.40
2:I:920:TRP:CD1	2:I:920:TRP:N	2.88	0.40
3:N:58:LEU:N	3:N:68:LYS:NZ	2.66	0.40
2:B:131:ASN:O	2:B:292:LYS:NZ	2.45	0.40
2:B:197:GLU:HB3	2:B:198:PHE:CD1	2.56	0.40
2:B:657:PHE:CD1	2:B:657:PHE:N	2.89	0.40
1:C:451:ARG:HD2	1:C:473:THR:O	2.21	0.40
2:D:305:ALA:HB1	2:D:393:GLU:O	2.22	0.40
2:D:412:GLN:HG3	2:D:451:ILE:HG12	2.02	0.40
2:D:836:ILE:HD12	2:D:836:ILE:HA	1.76	0.40
3:F:57:TRP:CZ2	3:F:70:LYS:HE3	2.56	0.40
1:H:97:ASN:O	1:H:101:ARG:HG3	2.20	0.40
2:M:734:LEU:H	2:M:757:THR:HG22	1.86	0.40
1:A:427:GLU:H	1:A:427:GLU:HG2	1.75	0.40
1:A:448:LEU:O	1:A:450:LYS:HE3	2.21	0.40
1:C:409:ARG:HH21	1:C:410:THR:CG2	2.35	0.40
2:D:180:ASN:HB2	2:D:258:SER:HB3	2.02	0.40
3:F:58:LEU:HD11	3:F:120:TYR:CE2	2.56	0.40
3:F:73:VAL:HG12	3:F:80:PHE:HB3	2.03	0.40
1:H:196:ALA:HB2	1:H:477:TRP:HA	2.03	0.40
3:J:23:VAL:O	3:J:34:ASP:HA	2.22	0.40
3:J:75:TYR:O	3:J:78:ARG:HD3	2.20	0.40
2:B:116:SER:HB2	2:B:124:TYR:CE2	2.56	0.40
2:B:461:ILE:O	2:B:479:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:973:SER:OG	2:B:975:ARG:NH1	2.55	0.40
3:E:87:ASP:HA	3:E:94:LYS:HD2	2.04	0.40
1:H:116:VAL:HB	1:H:120:SER:O	2.21	0.40
1:H:144:VAL:O	1:H:148:ILE:HG12	2.21	0.40
2:I:349:GLN:HE21	2:I:349:GLN:HB3	1.71	0.40
2:I:753:MET:HE2	2:I:762:GLY:CA	2.51	0.40
1:L:142:GLU:OE2	1:L:476:TRP:CD2	2.74	0.40
1:L:476:TRP:CE2	1:L:477:TRP:CD1	3.08	0.40
2:M:665:VAL:HG13	2:M:704:LEU:HD13	2.03	0.40
2:B:582:ILE:HD13	2:B:656:PHE:CD1	2.57	0.40
2:B:713:THR:CG2	2:B:714:LYS:N	2.85	0.40
2:M:234:LYS:NZ	2:M:351:ASP:OD2	2.55	0.40
2:M:731:VAL:CG2	2:M:761:VAL:HG12	2.50	0.40
2:M:741:ILE:HG13	2:M:756:ILE:HG12	2.03	0.40
2:M:760:PRO:HB2	2:M:799:ASN:ND2	2.36	0.40
3:N:68:LYS:HZ2	3:N:69:LEU:C	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/480 (100%)	453 (95%)	24 (5%)	2 (0%)	34	66
1	C	479/480 (100%)	452 (94%)	24 (5%)	3 (1%)	25	56
1	H	479/480 (100%)	441 (92%)	35 (7%)	3 (1%)	25	56
1	L	479/480 (100%)	436 (91%)	41 (9%)	2 (0%)	34	66
2	B	937/984 (95%)	880 (94%)	49 (5%)	8 (1%)	17	46
2	D	941/984 (96%)	885 (94%)	54 (6%)	2 (0%)	47	78
2	I	945/984 (96%)	882 (93%)	58 (6%)	5 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	946/984 (96%)	893 (94%)	52 (6%)	1 (0%)	51	81
3	E	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
3	F	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
3	J	144/148 (97%)	136 (94%)	6 (4%)	2 (1%)	11	34
3	N	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	53
4	G	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	1
4	K	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	O	8/10 (80%)	6 (75%)	0	2 (25%)	0	0
4	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	6293/6488 (97%)	5895 (94%)	366 (6%)	32 (0%)	29	61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	38	LYS
2	B	659	ASN
2	B	866	GLY
2	B	920	TRP
1	C	371	ALA
1	C	372	CYS
2	D	848	TYR
1	H	124	TYR
2	I	577	ASN
3	N	33	GLU
1	A	120	SER
1	C	120	SER
2	I	578	LEU
3	J	125	ASP
4	O	2	GLY
4	O	3	GLY
2	B	658	LYS
1	H	125	SER
2	I	579	GLN
3	J	27	ILE
1	L	417	SER
2	B	95	SER
2	M	813	LYS
1	A	124	TYR
2	B	867	GLU

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Mol	Chain	Res	Type
2	D	362	PRO
1	H	120	SER
2	I	713	THR
1	L	378	SER
4	G	3	GLY
2	I	573	LEU
2	B	362	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/392 (100%)	370 (94%)	23 (6%)	19	49
1	C	393/392 (100%)	377 (96%)	16 (4%)	30	64
1	H	393/392 (100%)	367 (93%)	26 (7%)	16	44
1	L	393/392 (100%)	356 (91%)	37 (9%)	8	26
2	B	793/836 (95%)	743 (94%)	50 (6%)	18	46
2	D	797/836 (95%)	738 (93%)	59 (7%)	13	37
2	I	799/836 (96%)	753 (94%)	46 (6%)	20	50
2	M	800/836 (96%)	754 (94%)	46 (6%)	20	50
3	E	122/124 (98%)	116 (95%)	6 (5%)	25	57
3	F	122/124 (98%)	117 (96%)	5 (4%)	30	64
3	J	122/124 (98%)	112 (92%)	10 (8%)	11	33
3	N	122/124 (98%)	114 (93%)	8 (7%)	16	44
All	All	5249/5408 (97%)	4917 (94%)	332 (6%)	18	46

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	27	SER
1	A	49	TYR

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Mol	Chain	Res	Type
1	A	55	SER
1	A	108	ARG
1	A	139	ASP
1	A	169	LEU
1	A	177	GLN
1	A	222	LYS
1	A	227	LEU
1	A	257	TYR
1	A	274	ASP
1	A	276	ASP
1	A	278	LYS
1	A	320	PHE
1	A	358	ARG
1	A	375	SER
1	A	383	LYS
1	A	384	LEU
1	A	397	TYR
1	A	428	SER
1	A	431	THR
1	A	459	ARG
2	B	45	THR
2	B	51	LYS
2	B	60	VAL
2	B	87	ILE
2	B	94	LEU
2	B	97	THR
2	B	99	GLN
2	B	108	PRO
2	B	155	SER
2	B	170	ARG
2	B	173	LYS
2	B	259	LEU
2	B	260	SER
2	B	262	ASN
2	B	282	MET
2	B	317	GLN
2	B	333	SER
2	B	410	THR
2	B	426	GLU
2	B	436	SER
2	B	490	GLN
2	B	498	THR

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Mol	Chain	Res	Type
2	B	518	MET
2	B	567	SER
2	B	602	MET
2	B	623	LEU
2	B	645	THR
2	B	657	PHE
2	B	658	LYS
2	B	670	ARG
2	B	675	GLN
2	B	704	LEU
2	B	706	ILE
2	B	707	SER
2	B	757	THR
2	B	798	MET
2	B	809	ASN
2	B	816	SER
2	B	824	ARG
2	B	829	MET
2	B	832	ARG
2	B	858	ASN
2	B	870	THR
2	B	915	ASP
2	B	916	LEU
2	B	959	ASP
2	B	968	THR
2	B	974	ARG
2	B	980	LEU
2	B	981	MET
1	C	15	ASP
1	C	27	SER
1	C	41	TYR
1	C	49	TYR
1	C	144	VAL
1	C	225	CYS
1	C	320	PHE
1	C	324	GLU
1	C	367	ILE
1	C	397	TYR
1	C	405	SER
1	C	414	LYS
1	C	431	THR
1	C	434	GLU

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Mol	Chain	Res	Type
1	C	440	THR
1	C	459	ARG
2	D	58	SER
2	D	59	ASP
2	D	60	VAL
2	D	61	MET
2	D	74	SER
2	D	97	THR
2	D	99	GLN
2	D	171	LYS
2	D	173	LYS
2	D	183	VAL
2	D	184	GLN
2	D	195	GLN
2	D	208	GLU
2	D	235	LEU
2	D	282	MET
2	D	288	ASP
2	D	298	ARG
2	D	307	THR
2	D	313	ASN
2	D	319	ASN
2	D	333	SER
2	D	339	ARG
2	D	342	SER
2	D	366	MET
2	D	408	THR
2	D	413	SER
2	D	417	LYS
2	D	432	GLU
2	D	441	SER
2	D	477	LEU
2	D	518	MET
2	D	533	SER
2	D	541	THR
2	D	543	THR
2	D	546	ASN
2	D	557	ARG
2	D	558	SER
2	D	581	VAL
2	D	586	LYS
2	D	594	THR

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Mol	Chain	Res	Type
2	D	613	ARG
2	D	675	GLN
2	D	692	MET
2	D	702	ILE
2	D	713	THR
2	D	720	LEU
2	D	782	SER
2	D	785	LEU
2	D	828	VAL
2	D	829	MET
2	D	832	ARG
2	D	867	GLU
2	D	870	THR
2	D	893	ASP
2	D	906	LYS
2	D	915	ASP
2	D	932	SER
2	D	966	GLU
2	D	981	MET
3	E	3	ASN
3	E	4	ASP
3	E	13	GLU
3	E	22	THR
3	E	60	ASP
3	E	93	SER
3	F	4	ASP
3	F	30	LYS
3	F	75	TYR
3	F	92	GLU
3	F	101	LYS
1	H	1	CYS
1	H	27	SER
1	H	49	TYR
1	H	74	ASP
1	H	125	SER
1	H	137	LYS
1	H	140	THR
1	H	177	GLN
1	H	207	VAL
1	H	222	LYS
1	H	229	GLU
1	H	233	ARG

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Mol	Chain	Res	Type
1	H	260	SER
1	H	272	LYS
1	H	278	LYS
1	H	287	LYS
1	H	320	PHE
1	H	321	THR
1	H	348	GLU
1	H	382	ASP
1	H	383	LYS
1	H	387	ILE
1	H	397	TYR
1	H	401	MET
1	H	457	SER
1	H	459	ARG
2	I	56	ARG
2	I	105	ASP
2	I	171	LYS
2	I	190	ARG
2	I	195	GLN
2	I	200	MET
2	I	259	LEU
2	I	266	ASP
2	I	275	SER
2	I	278	SER
2	I	282	MET
2	I	318	LYS
2	I	366	MET
2	I	376	LEU
2	I	395	LEU
2	I	406	LEU
2	I	408	THR
2	I	423	LEU
2	I	436	SER
2	I	441	SER
2	I	455	ARG
2	I	516	GLN
2	I	518	MET
2	I	554	LYS
2	I	571	SER
2	I	578	LEU
2	I	588	ARG
2	I	675	GLN

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Mol	Chain	Res	Type
2	I	678	SER
2	I	692	MET
2	I	753	MET
2	I	765	LYS
2	I	767	GLN
2	I	779	VAL
2	I	801	LYS
2	I	803	GLN
2	I	829	MET
2	I	844	ILE
2	I	873	GLU
2	I	879	THR
2	I	902	LYS
2	I	908	ARG
2	I	915	ASP
2	I	919	ARG
2	I	930	LYS
2	I	981	MET
3	J	4	ASP
3	J	27	ILE
3	J	60	ASP
3	J	69	LEU
3	J	82	THR
3	J	83	THR
3	J	92	GLU
3	J	96	LYS
3	J	105	LYS
3	J	132	THR
1	L	1	CYS
1	L	27	SER
1	L	49	TYR
1	L	74	ASP
1	L	108	ARG
1	L	121	ASP
1	L	137	LYS
1	L	144	VAL
1	L	145	TYR
1	L	146	LYS
1	L	169	LEU
1	L	177	GLN
1	L	188	ARG
1	L	227	LEU

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Mol	Chain	Res	Type
1	L	260	SER
1	L	266	ILE
1	L	271	SER
1	L	272	LYS
1	L	274	ASP
1	L	291	GLN
1	L	305	SER
1	L	320	PHE
1	L	322	GLN
1	L	328	LEU
1	L	331	GLU
1	L	379	THR
1	L	380	GLN
1	L	384	LEU
1	L	389	MET
1	L	397	TYR
1	L	424	GLN
1	L	427	GLU
1	L	428	SER
1	L	429	VAL
1	L	431	THR
1	L	459	ARG
1	L	473	THR
2	M	74	SER
2	M	87	ILE
2	M	155	SER
2	M	170	ARG
2	M	171	LYS
2	M	195	GLN
2	M	222	MET
2	M	236	LYS
2	M	310	SER
2	M	323	THR
2	M	387	LYS
2	M	390	LEU
2	M	415	LYS
2	M	421	TYR
2	M	426	GLU
2	M	441	SER
2	M	452	THR
2	M	462	MET
2	M	475	ASN

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Mol	Chain	Res	Type
2	M	490	GLN
2	M	516	GLN
2	M	524	MET
2	M	530	PHE
2	M	567	SER
2	M	571	SER
2	M	572	GLU
2	M	574	LEU
2	M	579	GLN
2	M	630	SER
2	M	648	SER
2	M	666	SER
2	M	675	GLN
2	M	692	MET
2	M	714	LYS
2	M	761	VAL
2	M	767	GLN
2	M	776	ARG
2	M	813	LYS
2	M	816	SER
2	M	829	MET
2	M	868	ASN
2	M	915	ASP
2	M	918	LYS
2	M	919	ARG
2	M	923	LYS
2	M	968	THR
3	N	4	ASP
3	N	30	LYS
3	N	31	GLU
3	N	68	LYS
3	N	70	LYS
3	N	82	THR
3	N	96	LYS
3	N	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	56	ASN
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	282	GLN
1	A	337	HIS
2	B	84	ASN
2	B	128	ASN
2	B	195	GLN
2	B	774	GLN
1	C	326	GLN
1	C	460	GLN
2	D	262	ASN
2	D	419	ASN
2	D	690	GLN
2	I	131	ASN
2	I	301	HIS
2	I	459	GLN
2	I	609	GLN
2	I	627	ASN
2	I	748	ASN
2	I	767	GLN
2	I	800	ASN
2	I	842	ASN
2	I	979	ASN
1	L	56	ASN
1	L	59	ASN
1	L	424	GLN
2	M	110	ASN
2	M	868	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	KR0	M	1985	-	26,26,26	1.24	2 (7%)	27,27,27	1.36	4 (14%)
5	KR0	I	1985	-	26,26,26	1.28	2 (7%)	27,27,27	1.32	4 (14%)
5	KR0	D	1985	-	26,26,26	1.25	2 (7%)	27,27,27	1.31	4 (14%)
5	KR0	B	1985	-	26,26,26	1.37	2 (7%)	27,27,27	1.14	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KR0	M	1985	-	-	8/26/26/26	-
5	KR0	I	1985	-	-	9/26/26/26	-
5	KR0	D	1985	-	-	10/26/26/26	-
5	KR0	B	1985	-	-	6/26/26/26	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1985	KR0	O4-C5	4.89	1.47	1.33
5	B	1985	KR0	O1-C7	4.58	1.46	1.33
5	I	1985	KR0	O1-C7	4.52	1.46	1.33
5	M	1985	KR0	O1-C7	4.41	1.46	1.33
5	D	1985	KR0	O1-C7	4.34	1.46	1.33
5	D	1985	KR0	O4-C5	4.20	1.45	1.33
5	I	1985	KR0	O4-C5	4.09	1.45	1.33
5	M	1985	KR0	O4-C5	4.03	1.45	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1985	KR0	O1-C7-C12	3.99	124.42	111.91
5	M	1985	KR0	O1-C7-C12	3.60	123.22	111.91
5	D	1985	KR0	O4-C5-C10	3.55	123.06	111.91
5	M	1985	KR0	O4-C5-C10	3.53	122.98	111.91
5	B	1985	KR0	O1-C7-C12	3.27	122.18	111.91
5	D	1985	KR0	O1-C7-C12	3.13	121.73	111.91
5	I	1985	KR0	O4-C5-C10	2.99	121.30	111.91
5	M	1985	KR0	O4-C5-O8	-2.91	116.25	123.59
5	D	1985	KR0	O4-C5-O8	-2.91	116.26	123.59
5	B	1985	KR0	O4-C5-C10	2.69	120.36	111.91
5	I	1985	KR0	O4-C5-O8	-2.49	117.30	123.59
5	I	1985	KR0	O1-C7-O9	-2.38	117.59	123.59
5	M	1985	KR0	O1-C7-O9	-2.25	117.92	123.59
5	B	1985	KR0	O1-C7-O9	-2.12	118.23	123.59
5	D	1985	KR0	C3-C2-C1	-2.06	106.84	113.70

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1985	KR0	O9-C7-O1-C1
5	B	1985	KR0	C12-C7-O1-C1
5	D	1985	KR0	O9-C7-O1-C1
5	D	1985	KR0	C12-C7-O1-C1
5	I	1985	KR0	O9-C7-O1-C1
5	I	1985	KR0	C12-C7-O1-C1
5	M	1985	KR0	O9-C7-O1-C1
5	M	1985	KR0	C12-C7-O1-C1
5	D	1985	KR0	C1-C2-C3-O4
5	I	1985	KR0	C1-C2-C3-O4
5	I	1985	KR0	C7-C12-C13-C17
5	M	1985	KR0	C1-C2-C3-O4
5	M	1985	KR0	C7-C12-C13-C17
5	I	1985	KR0	O1-C1-C2-C3
5	M	1985	KR0	O1-C1-C2-C3
5	I	1985	KR0	C12-C13-C17-C18
5	D	1985	KR0	C12-C13-C17-C18
5	I	1985	KR0	C10-C11-C4-C6
5	M	1985	KR0	C12-C13-C17-C18
5	D	1985	KR0	C7-C12-C13-C17
5	D	1985	KR0	O1-C1-C2-C3
5	B	1985	KR0	C1-C2-C3-O4
5	B	1985	KR0	C12-C13-C17-C18

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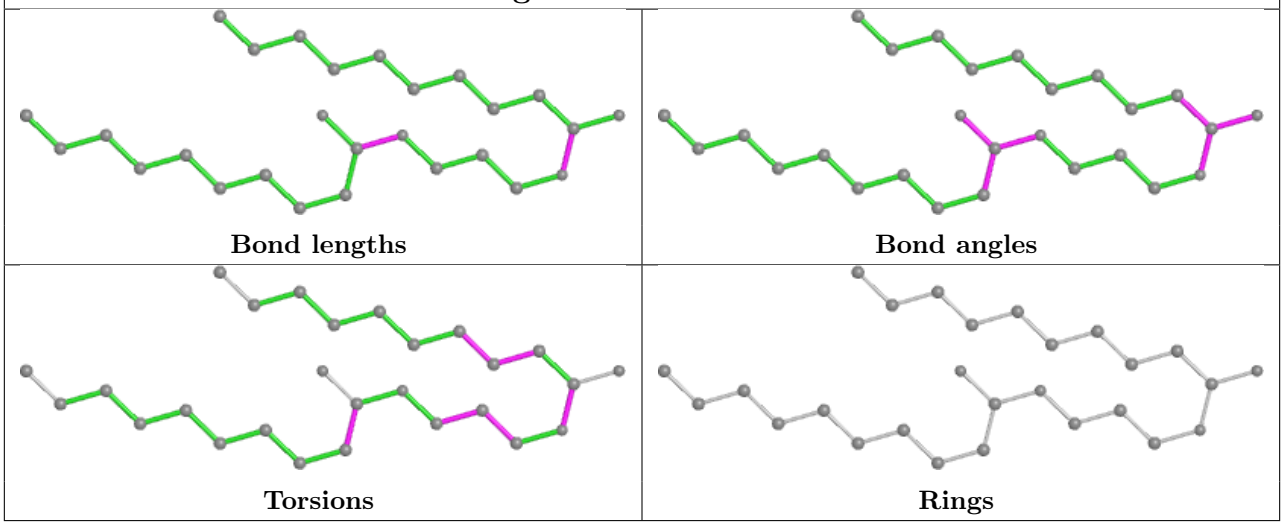
Mol	Chain	Res	Type	Atoms
5	D	1985	KR0	C17-C18-C19-C20
5	D	1985	KR0	C15-C14-C9-C8
5	M	1985	KR0	C11-C10-C5-O4
5	B	1985	KR0	O1-C1-C2-C3
5	D	1985	KR0	C11-C10-C5-O4
5	B	1985	KR0	C10-C11-C4-C6
5	M	1985	KR0	C11-C10-C5-O8
5	I	1985	KR0	C11-C10-C5-O4
5	I	1985	KR0	C11-C10-C5-O8
5	D	1985	KR0	C11-C10-C5-O8

There are no ring outliers.

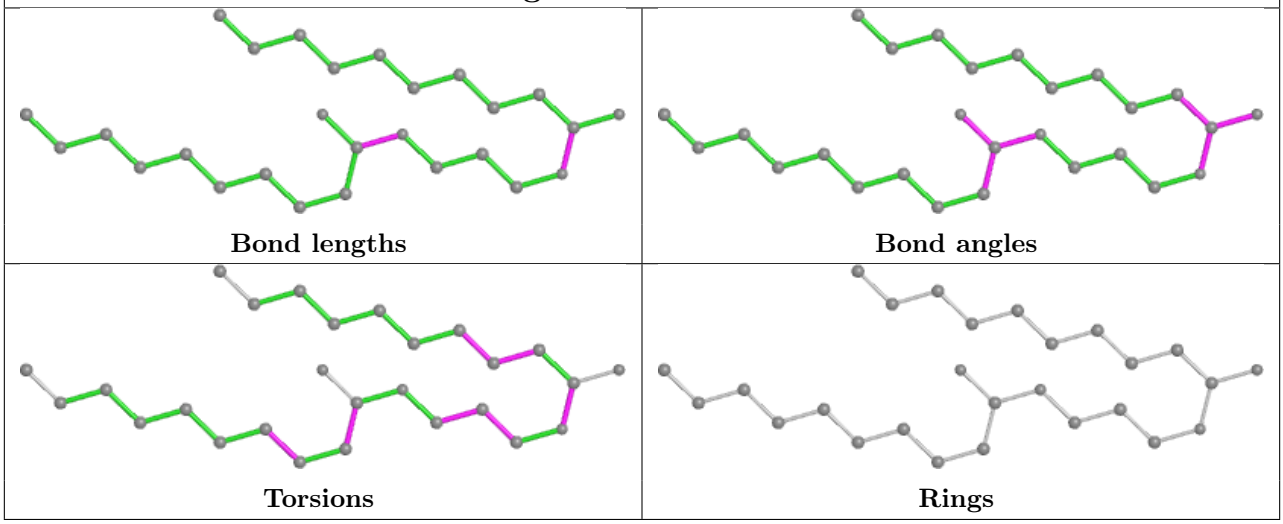
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

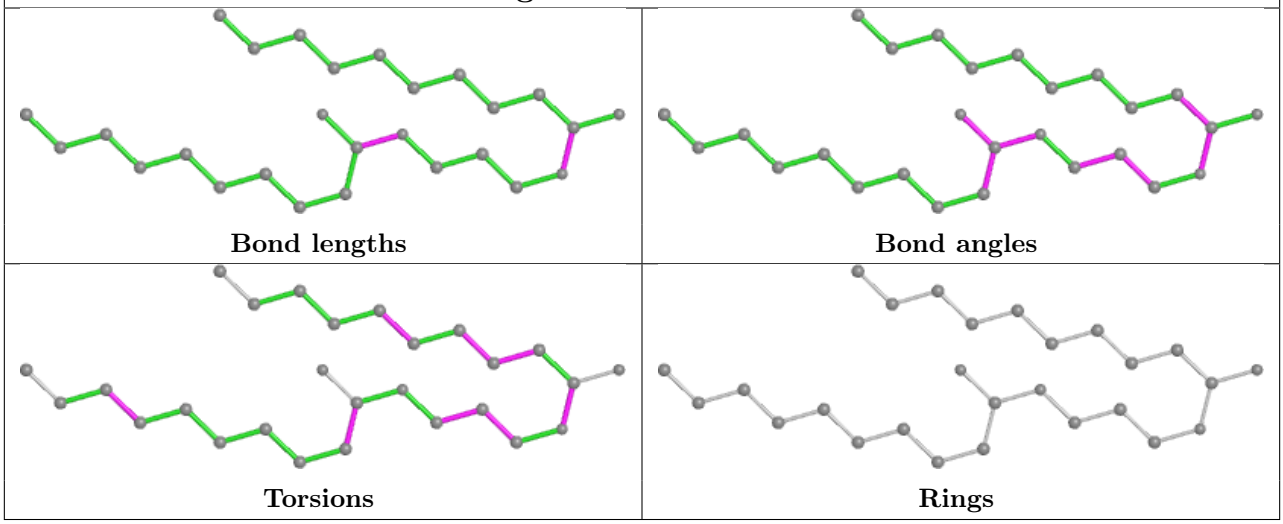
Ligand KR0 M 1985



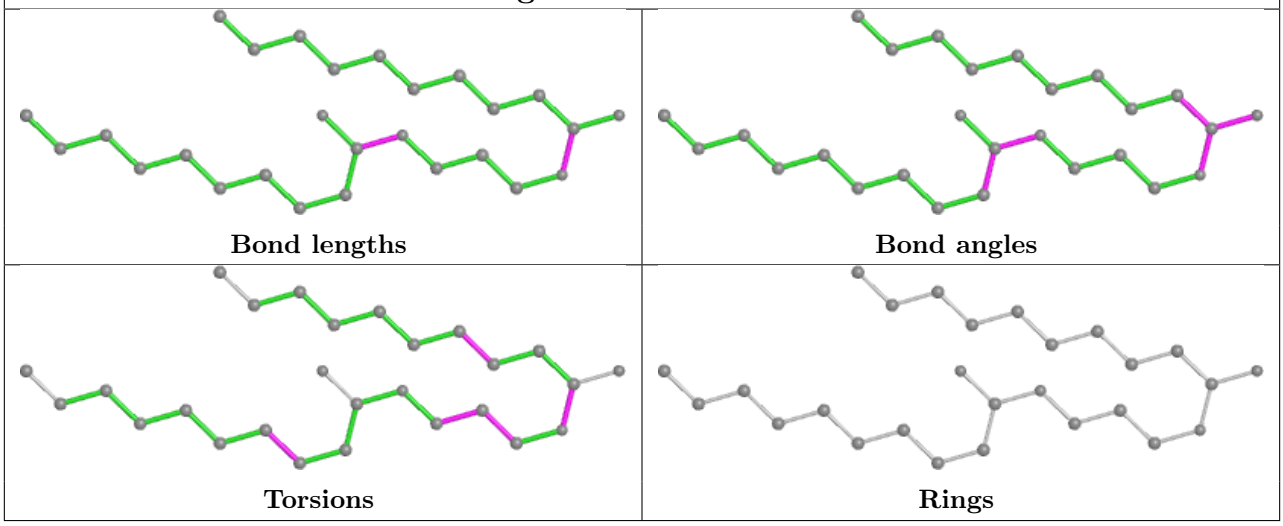
Ligand KR0 I 1985



Ligand KR0 D 1985



Ligand KR0 B 1985



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	480/480 (100%)	-0.24	2 (0%)	92	91	43, 66, 98, 161	0
1	C	480/480 (100%)	-0.32	1 (0%)	95	94	35, 57, 87, 116	0
1	H	480/480 (100%)	-0.09	6 (1%)	77	72	39, 68, 101, 166	0
1	L	480/480 (100%)	-0.02	7 (1%)	73	68	40, 77, 115, 171	0
2	B	941/984 (95%)	-0.21	7 (0%)	87	84	35, 60, 96, 135	0
2	D	945/984 (96%)	-0.29	8 (0%)	86	81	31, 50, 80, 154	0
2	I	947/984 (96%)	-0.28	7 (0%)	87	84	32, 52, 81, 160	0
2	M	948/984 (96%)	-0.30	9 (0%)	84	80	31, 51, 79, 172	0
3	E	146/148 (98%)	0.05	1 (0%)	87	84	47, 63, 90, 118	0
3	F	146/148 (98%)	0.36	8 (5%)	25	16	58, 75, 100, 117	0
3	J	146/148 (98%)	0.11	3 (2%)	63	54	56, 81, 108, 154	0
3	N	146/148 (98%)	0.33	9 (6%)	20	13	63, 86, 112, 137	0
4	G	10/10 (100%)	1.37	1 (10%)	7	4	37, 49, 63, 75	0
4	K	10/10 (100%)	1.47	0	100	100	39, 46, 64, 87	0
4	O	10/10 (100%)	1.13	1 (10%)	7	4	38, 51, 73, 88	0
4	P	10/10 (100%)	1.32	0	100	100	41, 50, 62, 96	0
All	All	6325/6488 (97%)	-0.18	70 (1%)	80	75	31, 59, 97, 172	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	866	GLY	11.6
2	M	866	GLY	8.8
1	A	372	CYS	7.2
1	L	372	CYS	7.1
1	H	372	CYS	6.5

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Mol	Chain	Res	Type	RSRZ
2	D	574	LEU	5.2
2	I	865	ASN	5.1
2	I	864	VAL	4.7
3	N	29	GLY	4.0
2	B	581	VAL	3.9
2	B	579	GLN	3.7
2	D	866	GLY	3.7
1	H	376	ALA	3.7
3	N	3	ASN	3.6
2	D	580	ASP	3.4
1	H	375	SER	3.4
3	J	148	PHE	3.3
2	M	865	ASN	3.3
2	D	173	LYS	3.2
2	M	864	VAL	3.2
1	L	376	ALA	3.2
2	I	867	GLU	3.2
2	B	984	PHE	3.1
1	A	371	ALA	3.1
2	M	37	GLU	3.1
2	D	573	LEU	2.9
3	N	148	PHE	2.9
3	N	38	ALA	2.9
1	H	194	ILE	2.9
3	F	28	ASP	2.8
3	F	25	ALA	2.7
1	L	336	PHE	2.7
2	I	733	SER	2.6
3	F	91	TYR	2.6
3	N	37	GLY	2.6
2	M	576	ASP	2.6
2	B	582	ILE	2.5
3	N	130	GLY	2.5
2	M	530	PHE	2.5
2	M	773	PRO	2.5
3	J	31	GLU	2.5
2	I	474	ILE	2.5
3	F	31	GLU	2.5
1	C	376	ALA	2.5
3	E	91	TYR	2.5
3	F	26	PHE	2.4
3	N	35	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	366	THR	2.3
3	J	133	TYR	2.3
3	F	137	GLY	2.3
1	L	160	ASP	2.3
2	B	679	LEU	2.3
2	B	773	PRO	2.3
3	F	30	LYS	2.2
4	G	1	GLY	2.2
1	L	375	SER	2.2
2	B	774	GLN	2.2
2	D	532	GLY	2.2
4	O	8	GLY	2.2
2	D	579	GLN	2.2
3	F	148	PHE	2.2
2	M	867	GLU	2.2
3	N	36	PHE	2.1
1	L	377	ALA	2.1
1	H	162	SER	2.1
2	M	733	SER	2.1
3	N	23	VAL	2.1
1	H	211	VAL	2.1
2	D	394	PHE	2.0
2	I	735	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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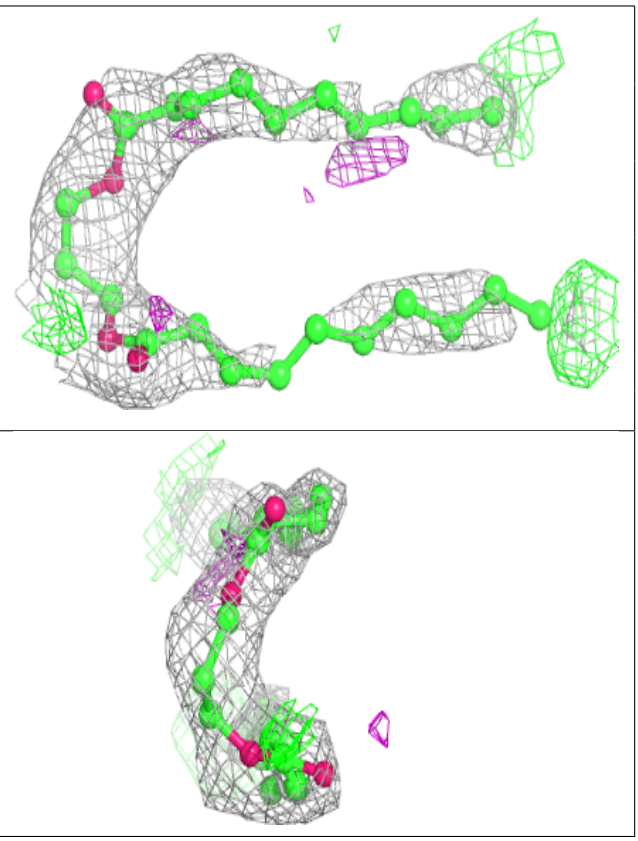
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	KR0	B	1985	27/27	0.82	0.41	52,73,83,89	0
5	KR0	D	1985	27/27	0.84	0.43	46,69,76,78	0
5	KR0	I	1985	27/27	0.85	0.36	43,54,77,87	0
5	KR0	M	1985	27/27	0.86	0.42	42,59,75,81	0
6	NA	M	1986	1/1	0.88	0.29	42,42,42,42	0
7	CA	I	1987	1/1	0.92	0.12	58,58,58,58	0
6	NA	I	1986	1/1	0.93	0.24	32,32,32,32	0
7	CA	M	1987	1/1	0.95	0.31	114,114,114,114	0
6	NA	B	1986	1/1	0.96	0.20	30,30,30,30	0
7	CA	D	1987	1/1	0.97	0.10	47,47,47,47	0
7	CA	B	1987	1/1	0.98	0.10	51,51,51,51	0
6	NA	D	1986	1/1	0.98	0.20	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

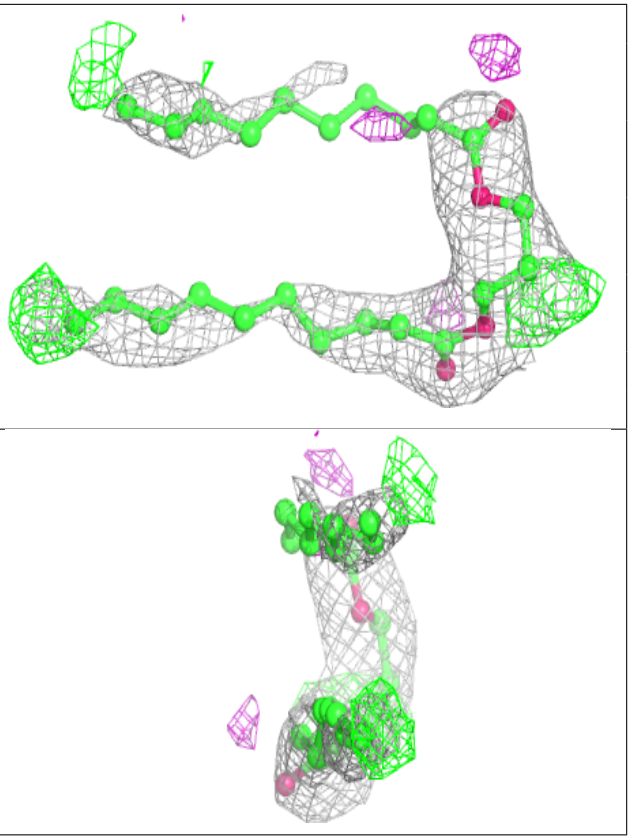
Electron density around KR0 B 1985:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



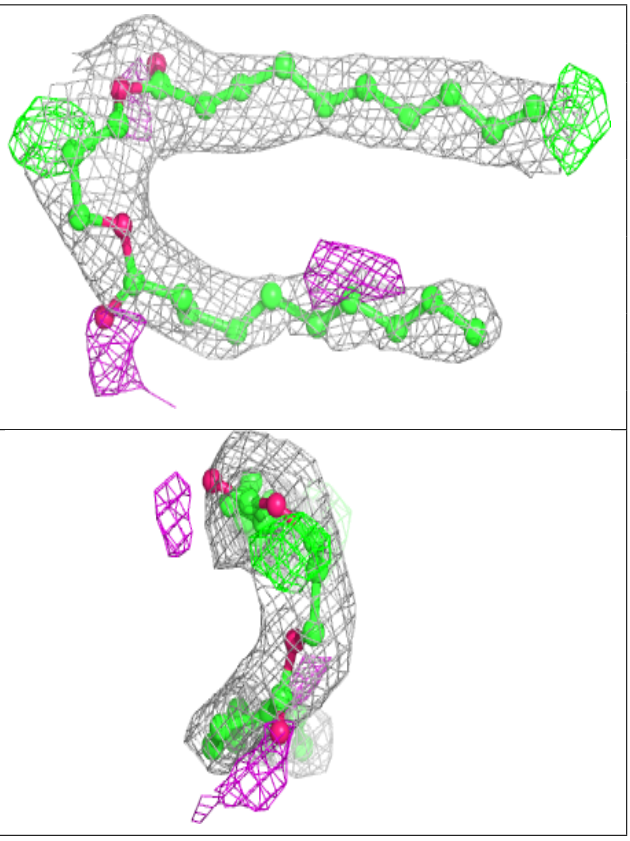
Electron density around KR0 D 1985:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



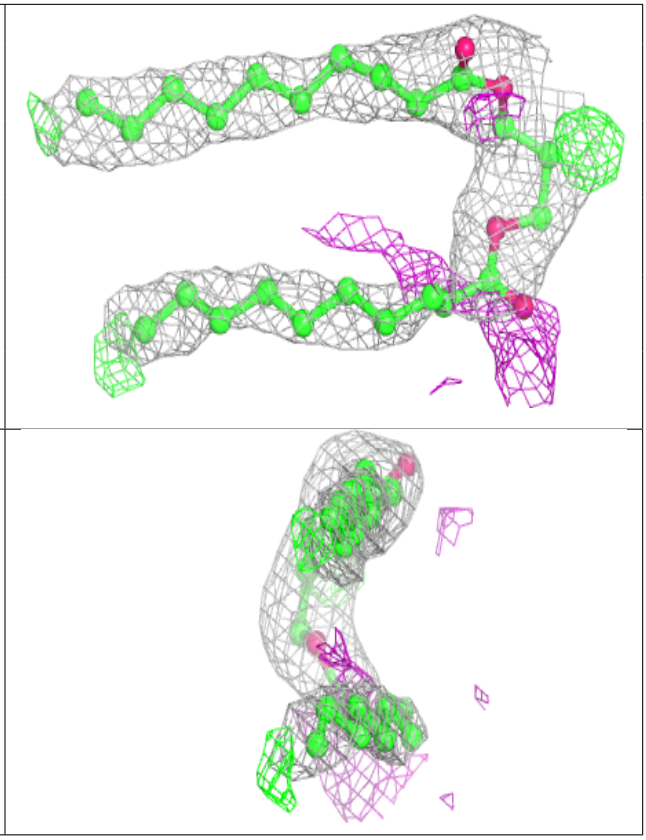
Electron density around KR0 I 1985:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around KR0 M 1985:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.